10/523,289

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=> file registry
FILE 'REGISTRY' ENTERED AT 17:33:14 ON 04 JAN 2007
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STRUCTURE FILE UPDATES:    3 JAN 2007  HIGHEST RN 916687-76-8
DICTIONARY FILE UPDATES:   3 JAN 2007  HIGHEST RN 916687-76-8

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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=> file caplus
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FILE COVERS 1907 - 4 Jan 2007  VOL 146 ISS 2
FILE LAST UPDATED: 3 Jan 2007  (20070103/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L65
L60          78 SEA FILE=CAPLUS ABB=ON  PLU=ON  KOGAMI K?/AU
L61           5 SEA FILE=CAPLUS ABB=ON  PLU=ON  HAYASHIZAKA N?/AU
L62         421 SEA FILE=CAPLUS ABB=ON  PLU=ON  SATAKE S?/AU
L63           2 SEA FILE=CAPLUS ABB=ON  PLU=ON  FUSEYA I?/AU
L64          37 SEA FILE=CAPLUS ABB=ON  PLU=ON  KAGANO H?/AU
L65           1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L60 AND L61 AND L62 AND L63
```

AND L64

```
=> d stat que L70
L60           78 SEA FILE=CAPLUS ABB=ON  PLU=ON  KOGAMI K?/AU
L61            5 SEA FILE=CAPLUS ABB=ON  PLU=ON  HAYASHIZAKA N?/AU
L62          421 SEA FILE=CAPLUS ABB=ON  PLU=ON  SATAKE S?/AU
L63            2 SEA FILE=CAPLUS ABB=ON  PLU=ON  FUSEYA I?/AU
L64           37 SEA FILE=CAPLUS ABB=ON  PLU=ON  KAGANO H?/AU
L66            2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L60 AND (L61 OR L62 OR L63 OR
                 L64)
L67            1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L61 AND (L62 OR L63 OR L64)
L68            4 SEA FILE=CAPLUS ABB=ON  PLU=ON  L62 AND (L63 OR L64)
L69            1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L63 AND L64
L70            5 SEA FILE=CAPLUS ABB=ON  PLU=ON  (L66 OR L67 OR L68 OR L69)


=> d stat que L71
L1             STR
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Structure attributes must be viewed using STN Express query preparation:
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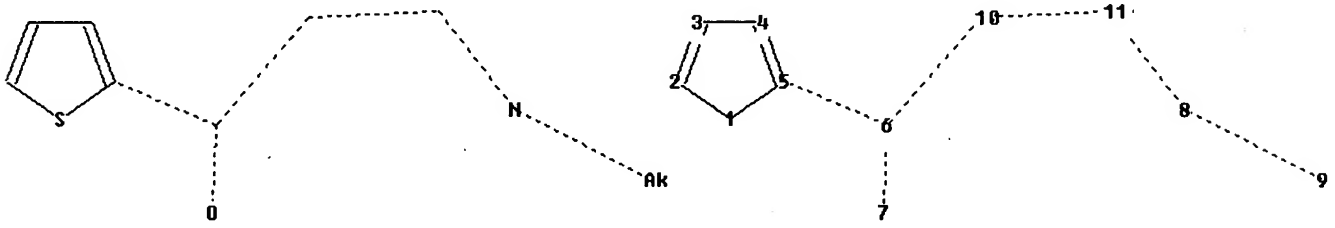


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chain nodes :
6  7  8  9  10  11
ring nodes :
1  2  3  4  5
chain bonds :
5-6  6-7  6-10  8-9  8-11  10-11
ring bonds :
1-2  1-5  2-3  3-4  4-5
exact/norm bonds :
1-2  1-5  2-3  3-4  4-5  5-6  6-7  6-10  8-9  8-11  10-11


Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:CLASS  10:Atom
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11:Atom

L3 676 SEA FILE=REGISTRY SSS FUL L1
L5 STR

Structure attributes must be viewed using STN Express query preparation:
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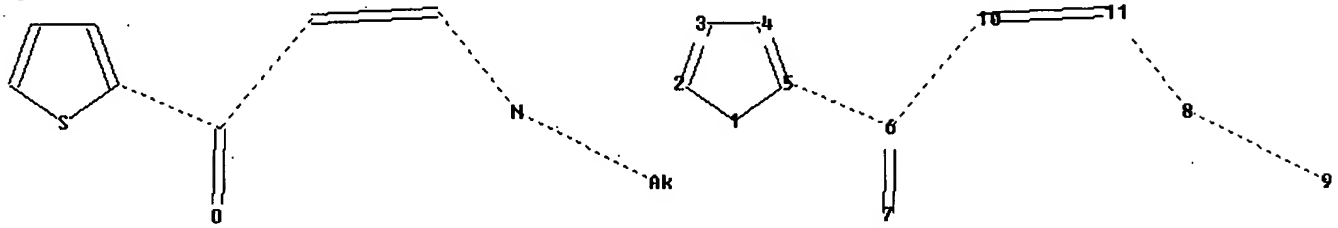
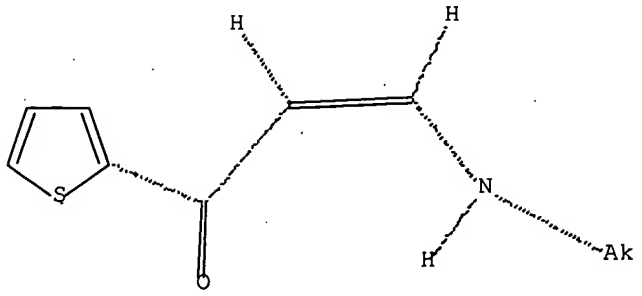


chain nodes :
6 7 8 9 10 11
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 10-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 10-11

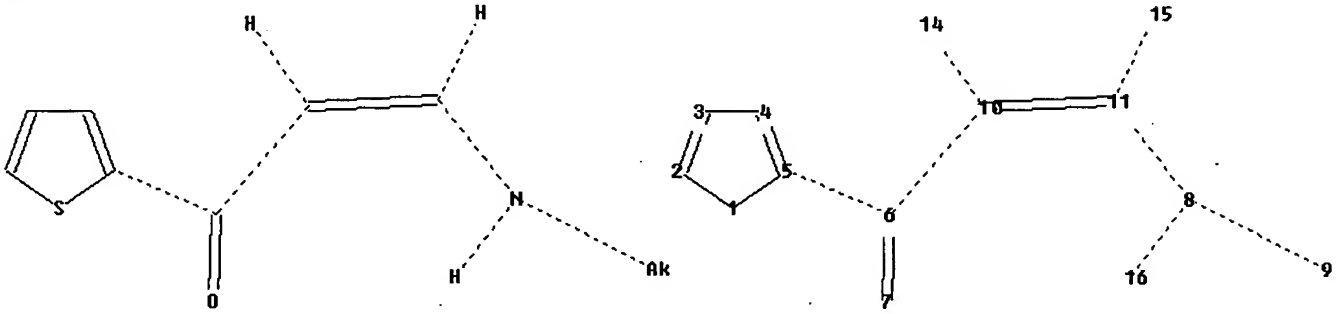
Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom

L7 159 SEA FILE=REGISTRY SUB=L3 SSS FUL L5
L8 124 SEA FILE=CAPLUS ABB=ON PLU=ON L7
L9 6 SEA FILE=REGISTRY ABB=ON PLU=ON L7 AND Z/BI
L10 2 SEA FILE=REGISTRY ABB=ON PLU=ON L7 AND 1Z/BI
L11 13 SEA FILE=REGISTRY ABB=ON PLU=ON L7 AND 2Z/BI
L13 18 SEA FILE=REGISTRY ABB=ON PLU=ON (L9 OR L10 OR L11)
L21 9 SEA FILE=CAPLUS ABB=ON PLU=ON L13
L22 273570 SEA FILE=CAPLUS ABB=ON PLU=ON ?STEREO?/BI

L25 6 SEA FILE=CAPLUS ABB=ON PLU=ON L8 AND L22
L37 STR



Structure attributes must be viewed using STN Express query preparation:
Uploading L37.str



chain nodes :
6 7 8 9 10 11 14 15 16
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 8-16 10-11 10-14 11-15
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 8-16 10-11 10-14 11-15

Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom 14:CLASS 15:CLASS 16:CLASS

L39 9 SEA FILE=REGISTRY SUB=L7 SSS FUL L37
L40 7 SEA FILE=CAPLUS ABB=ON PLU=ON L39
L60 78 SEA FILE=CAPLUS ABB=ON PLU=ON KOGAMI K?/AU
L61 5 SEA FILE=CAPLUS ABB=ON PLU=ON HAYASHIZAKA N?/AU
L62 421 SEA FILE=CAPLUS ABB=ON PLU=ON SATAKE S?/AU
L63 2 SEA FILE=CAPLUS ABB=ON PLU=ON FUSEYA I?/AU

```
L64           37 SEA FILE=CAPLUS ABB=ON  PLU=ON  KAGANO H?/AU
L71            1 SEA FILE=CAPLUS ABB=ON  PLU=ON  (L60 OR L61 OR L62 OR L63 OR
                 L64) AND (L21 OR L25 OR L40)


=> s L65 or L70 or L71
L77           5 L65 OR L70 OR L71

=> file marpat
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FILE CONTENT: 1961-PRESENT VOL 146 ISS 1 (20061229/ED)

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MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US       7138540 21 NOV 2006
DE 102005018025 02 NOV 2006
EP       1721898 15 NOV 2006
JP    2006310097 09 NOV 2006
WO    2006126581 30 NOV 2006
GB       2425654 01 NOV 2006
FR       2885527 17 NOV 2006
RU       2287007 10 NOV 2006
CA       2546348 11 NOV 2006

Expanded G-group definition display now available.

=> s L73
L78           1 L73

=> file wpix
FILE 'WPIX' ENTERED AT 17:34:38 ON 04 JAN 2007
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FILE LAST UPDATED:                    2 JAN 2007   <20070102/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE:     200701      <200701/DW>
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>>> FOR DETAILS ON THE NEW AND ENHANCED DERWENT WORLD PATENTS INDEX
    PLEASE SEE
```

http://www.stn-international.de/stndatabases/details/dwpi_r.html <<<

'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

```
=> d stat que L74
L60           78 SEA FILE=CAPLUS ABB=ON  PLU=ON  KOGAMI K?/AU
L61            5 SEA FILE=CAPLUS ABB=ON  PLU=ON  HAYASHIZAKA N?/AU
L62          421 SEA FILE=CAPLUS ABB=ON  PLU=ON  SATAKE S?/AU
L63            2 SEA FILE=CAPLUS ABB=ON  PLU=ON  FUSEYA I?/AU
L64           37 SEA FILE=CAPLUS ABB=ON  PLU=ON  KAGANO H?/AU
L66            2 SEA FILE=CAPLUS ABB=ON  PLU=ON  L60 AND (L61 OR L62 OR L63 OR
                 L64)
L67            1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L61 AND (L62 OR L63 OR L64)
L68            4 SEA FILE=CAPLUS ABB=ON  PLU=ON  L62 AND (L63 OR L64)
L69            1 SEA FILE=CAPLUS ABB=ON  PLU=ON  L63 AND L64
L74            4 SEA FILE=WPIX ABB=ON  PLU=ON  (L66 OR L67 OR L68 OR L69)


=> d stat que L75
L37              STR
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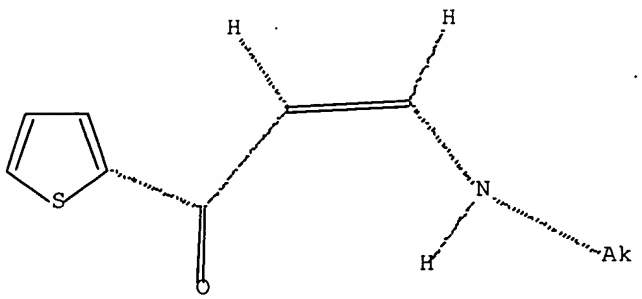

Structure attributes must be viewed using STN Express query preparation:
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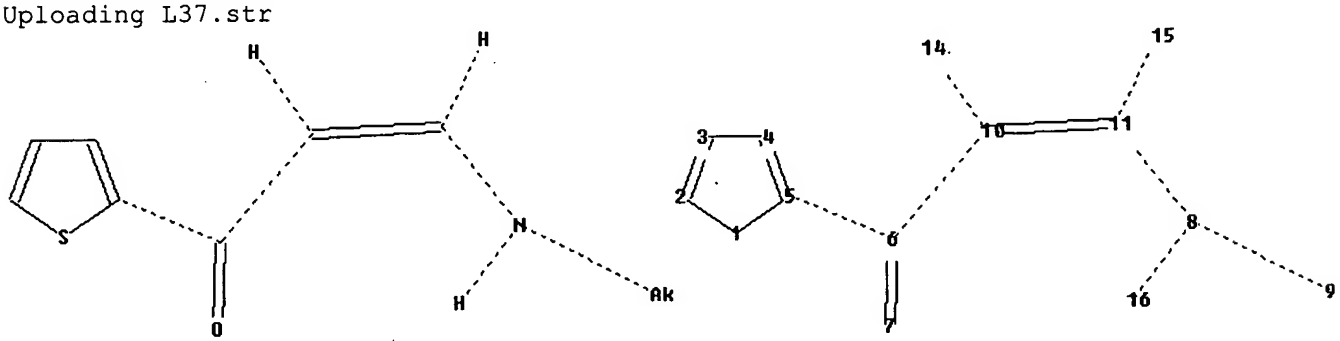


```
chain nodes :
6  7  8  9  10  11  14  15  16
ring nodes :
1  2  3  4  5
chain bonds :
5-6  6-7  6-10  8-9  8-11  8-16  10-11  10-14  11-15
ring bonds :
1-2  1-5  2-3  3-4  4-5
exact/norm bonds :
```

1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 8-16 10-11 10-14 11-15

Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom 14:CLASS 15:CLASS 16:CLASS

L57 1 SEA FILE=WPIX SSS FUL L37
L58 3 SEA FILE=WPIX ABB=ON PLU=ON L57/DCR
L59 3 SEA FILE=WPIX ABB=ON PLU=ON (RADOK2/DCR,DCN,DRN,DCRE OR 873835-0-0-0/DCR,DCN,DRN,DCRE)
L60 78 SEA FILE=CAPLUS ABB=ON PLU=ON KOGAMI K?/AU
L61 5 SEA FILE=CAPLUS ABB=ON PLU=ON HAYASHIZAKA N?/AU
L62 421 SEA FILE=CAPLUS ABB=ON PLU=ON SATAKE S?/AU
L63 2 SEA FILE=CAPLUS ABB=ON PLU=ON FUSEYA I?/AU
L64 37 SEA FILE=CAPLUS ABB=ON PLU=ON KAGANO H?/AU
L75 1 SEA FILE=WPIX ABB=ON PLU=ON (L60 OR L61 OR L62 OR L63 OR L64) AND (L58 OR L59)

=> s L74-L75
L79 4 (L74 OR L75)

=> => dup rem L77 L78 L79
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PROCESSING COMPLETED FOR L77
PROCESSING COMPLETED FOR L78
PROCESSING COMPLETED FOR L79
L80 5 DUP REM L77 L78 L79 (5 DUPLICATES REMOVED)
ANSWERS '1-5' FROM FILE CAPLUS

=> d ibib abs hitind hitstr L80 1-5

L80 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2005:564653 CAPLUS Full-text
DOCUMENT NUMBER: 143:97257
TITLE: Process for preparation of 2-acylthiophene derivatives
INVENTOR(S): Bando, Seiji; ***Satake, Syuzo; Kagano, Hirokazu***
PATENT ASSIGNEE(S): Sumitomo Seika Chemicals Co., Ltd., Japan
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005058866	A1	20050630	WO 2004-JP18569		20041213
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2544286	A1	20050630	CA 2004-2544286		20041213
EP 1695972	A1	20060830	EP 2004-806930		20041213
R: CH, DE, ES, FR, GB, IT, LI					
CN 1886396	A	20061227	CN 2004-80035125		20041213
PRIORITY APPLN. INFO.:			JP 2003-419362	A	20031217
			WO 2004-JP18569	W	20041213

OTHER SOURCE(S): CASREACT 143:97257; MARPAT 143:97257

AB This invention pertains to a method for producing 2-acylthiophene compds., characterized by reacting a thiophene compound with an acid anhydride or an acid halide in the presence of a solid acid catalyst at a temperature lower than 75 °C in the absence of any solvent. This invention provides a convenient method to prepare 2-acylthiophene derivs. with reduction of 3-acylthiophene byproduct.

IC ICM C07D333-22
ICS A61K031-381; C07B061-00
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L80 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2004:162681 CAPLUS Full-text
DOCUMENT NUMBER: 140:199199
TITLE: Process for preparation of N-monoalkyl-3-hydroxy-3-(2-thienyl)propanamines
INVENTOR(S): *Kogami, Kenji; Hayashizaka, Noriyuki ; Satake, Syuzo; Fuseya, Ichiro; Kagano, Hirokazu*
PATENT ASSIGNEE(S): Sumitomo Seika Chemicals Co., Ltd., Japan
SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

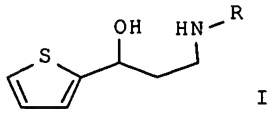
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004016603	A1	20040226	WO 2003-JP8950	20030715
W: CA, CN, JP, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2493776	A1	20040226	CA 2003-2493776	20030715
EP 1541569	A1	20050615	EP 2003-741391	20030715

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK

CN 1671686	A	20050921	CN 2003-818466		20030715
US 2005240030	A1	20051027	US 2005-523287		20050203
PRIORITY APPLN. INFO.:			JP 2002-229204	A	20020806
			WO 2003-JP8950	W	20030715

OTHER SOURCE(S): MARPAT 140:199199

GI



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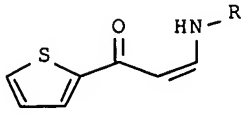


II

AB This invention pertains to a method for producing N-monoalkyl-3-hydroxy-3- (2-thienyl)propanamines with general formula of I [where R = alkyl], which comprises reduction of II with NaBH4 or Na(CN)H3. For example, β-oxo-β-(2-thienyl)propanal sodium salt was treated with MeNH2 in MeOH, followed by the addition of aqueous NaOH to give (Z)-N-methyl-3-oxo-3-(2- thienyl)-1-propenamine (74.8%). The propenamine was treated with NaBH4 in PhMe in the presence of AcOH to afford the title compound N-methyl-3-hydroxy-3-(2-thienyl)-1-propanamine (75.0%). By the process, an N-monoalkyl-3-hydroxy-3-(2-thienyl)propanamine useful as an intermediate for various medicines can be industrially and easily produced at low cost.

IC ICM C07D333-20
ICS C07D333-22

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 45

IT ***663603-70-1P***
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (thienyl)propanamines via reduction reaction)

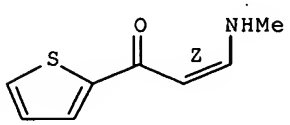
IT 74-89-5, Methylamine, reactions 75-04-7, Ethylamine, reactions 107-10-8, Propylamine, reactions 109-73-9, Butylamine, reactions 130371-57-2 ***663603-71-2*** ***663603-72-3*** ***663603-73-4***
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (thienyl)propanamines via reduction reaction)

IT ***663603-70-1P***
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (thienyl)propanamines via reduction reaction)

RN 663603-70-1 CAPLUS

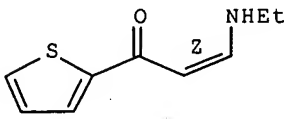
CN 2-Propen-1-one, 3-(methylamino)-1-(2-thienyl)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



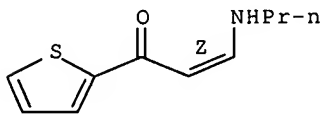
IT *663603-71-2 663603-72-3 663603-73-4*
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (thienyl)propanamines via reduction reaction)
RN 663603-71-2 CAPLUS
CN 2-Propen-1-one, 3-(ethylamino)-1-(2-thienyl)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



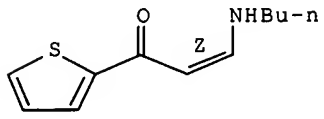
RN 663603-72-3 CAPLUS
CN 2-Propen-1-one, 3-(propylamino)-1-(2-thienyl)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 663603-73-4 CAPLUS
CN 2-Propen-1-one, 3-(butylamino)-1-(2-thienyl)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L80 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2003:391027 CAPLUS Full-text
DOCUMENT NUMBER: 138:401595
TITLE: Method for purification of 3-methylthiophene-2-carboxaldehyde
INVENTOR(S): ***Satake, Shuzo***; Hayashisaka, Yoshiyuki; ***Kagano, Hirokazu***
PATENT ASSIGNEE(S): Sumitomo Seika Chemicals Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003146984	A	20030521	JP 2001-346479	20011112

PRIORITY APPLN. INFO.: JP 2001-346479 20011112
OTHER SOURCE(S): CASREACT 138:401595

AB The title method comprises reacting a mixture of 3-methylthiophene-2-carboxaldehyde (I) and 3-methylthiophene-5-carboxaldehyde with hydrazine, separating N,N'-bis(3-methylthiophene-2-ylmethylene)hydrazine (II) and hydrolyzing II in the presence of an acid. I with 99.5% purity was obtained by the title method.

IC ICM C07D333-22
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))

L80 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2003:368908 CAPLUS Full-text
DOCUMENT NUMBER: 138:368753
TITLE: Preparation of 2,3-dimethylthiophene from 3-methylthiophene-2-carbaldehyde and 3-methylthiophene-5-carbaldehyde
INVENTOR(S): ***Satake, Shuzo***; Hayashizaka, Tokuyuki; ***Kagano, Hirokazu***
PATENT ASSIGNEE(S): Sumitomo Seika Chemicals Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003137882	A	20030514	JP 2001-340789	20011106

PRIORITY APPLN. INFO.: JP 2001-340789 20011106
OTHER SOURCE(S): CASREACT 138:368753

AB 2,3-Dimethylthiophene (I) is prepared by treatment of a mixture of 3-methylthiophene-2-carbaldehyde (II) and 3-methylthiophene-5-carbaldehyde (III) with NH2NH2, separating N,N'-bis(3-methylthiophen-2-ylmethylene)hydrazine (IV) from the reaction mixture, and reduction of IV with NH2NH2 in the presence of metal hydroxide. Thus, a II-III mixture was reacted with NH2NH2.H2O in MePh at 60° for 2 h to give 55% IV, which was treated with NH2NH2.H2O and NaOH in triethylene glycol at 130° for 4 h to afford 46.7% (based on the II-III mixture) I with 99.2% purity.

IC ICM C07D333-10
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))

L80 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:235913 CAPLUS Full-text
DOCUMENT NUMBER: 136:279219
TITLE: Process for preparing 4'-bromomethyl-2-cyanobiphenyl
INVENTOR(S): ***Satake, Shuzo***; Sato, Naoko; Takatori, Junichi; ***Kogami, Kenji***; Iida, Yukio
PATENT ASSIGNEE(S): Sumitomo Seika Chemicals Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002088044	A	20020327	JP 2000-279886	20000914

PRIORITY APPLN. INFO.: JP 2000-279886 20000914
OTHER SOURCE(S): CASREACT 136:279219

AB 4'-Bromomethyl-2-cyanobiphenyl (I) is prepared by reaction of 4'-methyl-2-cyanobiphenyl with bromine in the presence of a radical initiator under reduced pressure (25 KPa to 80 KPa). I is an intermediate for cardiovascular agents. I was prepared in 78.8% yield by the title process, vs. 40.4% yield in a reference process.

IC ICM C07C253-30
ICS C07C255-50
CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

=> file registry
FILE 'REGISTRY' ENTERED AT 17:35:54 ON 04 JAN 2007
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DICTIONARY FILE UPDATES: 3 JAN 2007 HIGHEST RN 916687-76-8

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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=> file caplus
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FILE COVERS 1907 - 4 Jan 2007 VOL 146 ISS 2
FILE LAST UPDATED: 3 Jan 2007 (20070103/ED)

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http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L21
L1 STR

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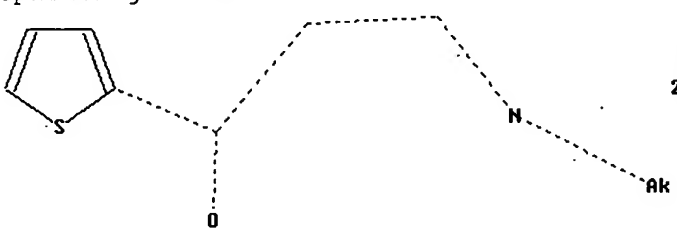

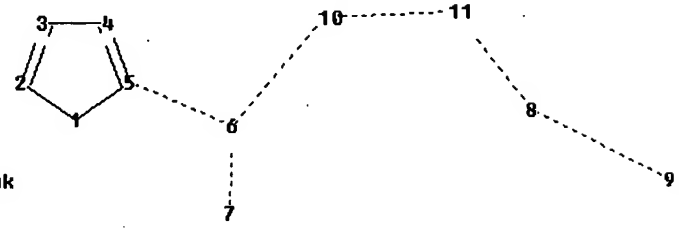

chain nodes :
6 7 8 9 10 11
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 10-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 10-11

Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom

L3 676 SEA FILE=REGISTRY SSS FUL L1
L5 STR

Structure attributes must be viewed using STN Express query preparation:
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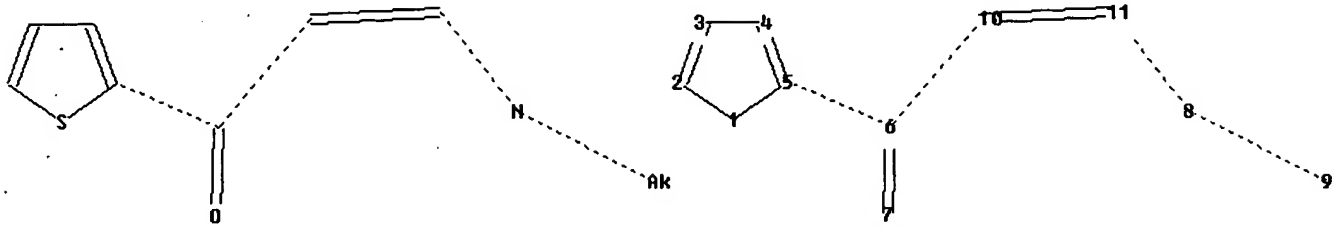

chain nodes :
6 7 8 9 10 11
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 10-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 10-11

Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom

```
L7          159 SEA FILE=REGISTRY SUB=L3 SSS FUL L5
L9            6 SEA FILE=REGISTRY ABB=ON  PLU=ON  L7 AND Z/BI
L10           2 SEA FILE=REGISTRY ABB=ON  PLU=ON  L7 AND 1Z/BI
L11          13 SEA FILE=REGISTRY ABB=ON  PLU=ON  L7 AND 2Z/BI
L13          18 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L9 OR L10 OR L11)
L21           9 SEA FILE=CAPLUS ABB=ON  PLU=ON  L13
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```
=> d stat que L25
L1              STR
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Structure attributes must be viewed using STN Express query preparation:
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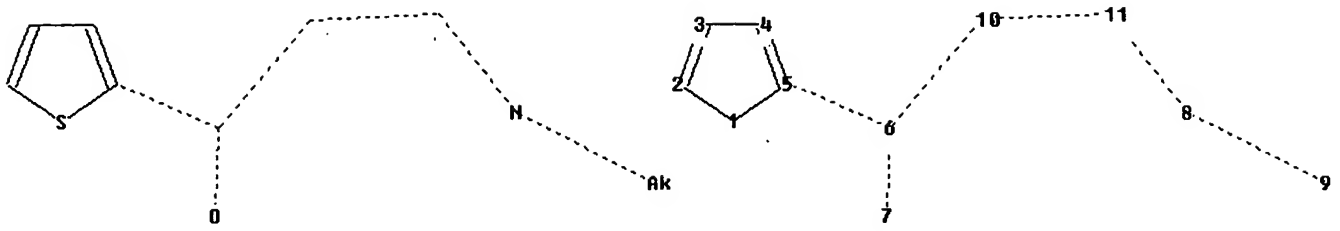

chain nodes :
6 7 8 9 10 11
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 10-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 10-11

Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom

L3 676 SEA FILE=REGISTRY SSS FUL L1
L5 STR

Structure attributes must be viewed using STN Express query preparation:
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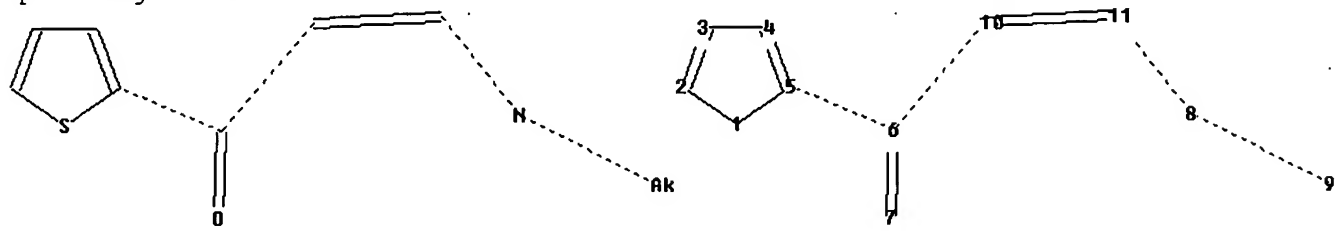


chain nodes :
6 7 8 9 10 11
ring nodes :

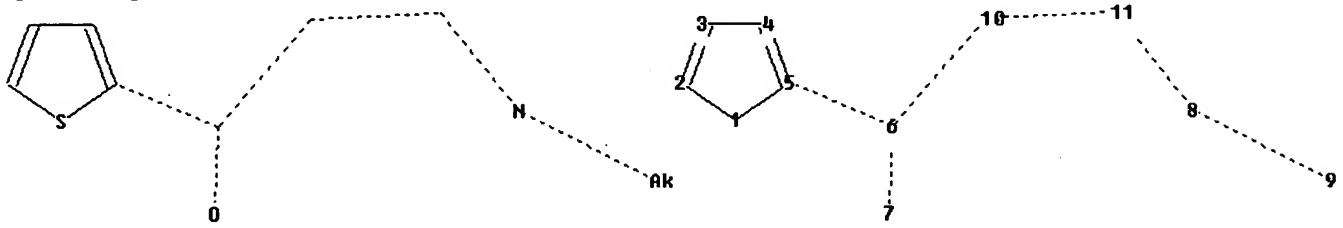
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 10-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 10-11

Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom

L7   159 SEA FILE=REGISTRY SUB=L3 SSS FUL L5
L8   124 SEA FILE=CAPLUS ABB=ON PLU=ON L7
L22   273570 SEA FILE=CAPLUS ABB=ON PLU=ON ?STEREO?/BI
L25   6 SEA FILE=CAPLUS ABB=ON PLU=ON L8 AND L22

=> d stat que L40
L1   STR

Structure attributes must be viewed using STN Express query preparation:
Uploading L1.str



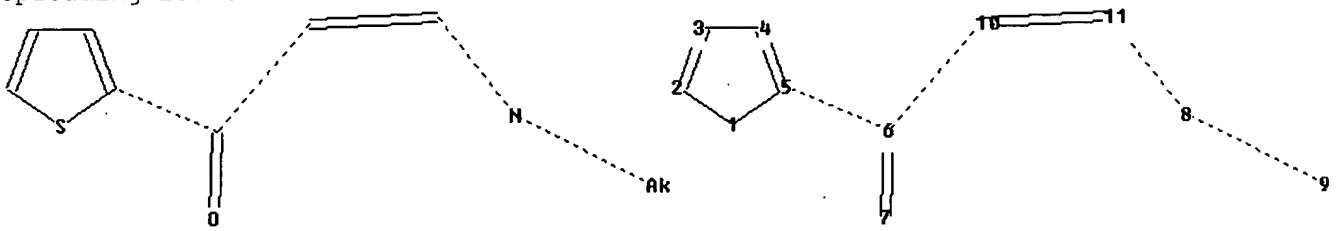
chain nodes :
6 7 8 9 10 11
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 10-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 10-11

Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom

L3 676 SEA FILE=REGISTRY SSS FUL L1
L5 STR

Structure attributes must be viewed using STN Express query preparation:
Uploading L5.str

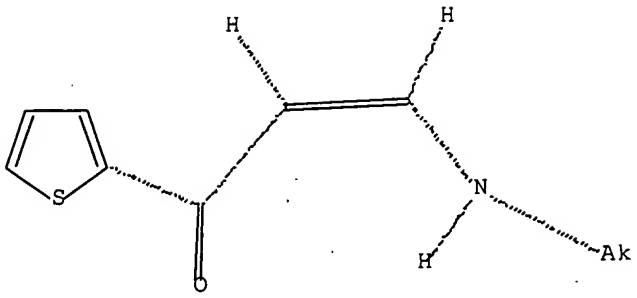


chain nodes :
6 7 8 9 10 11
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 10-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 10-11

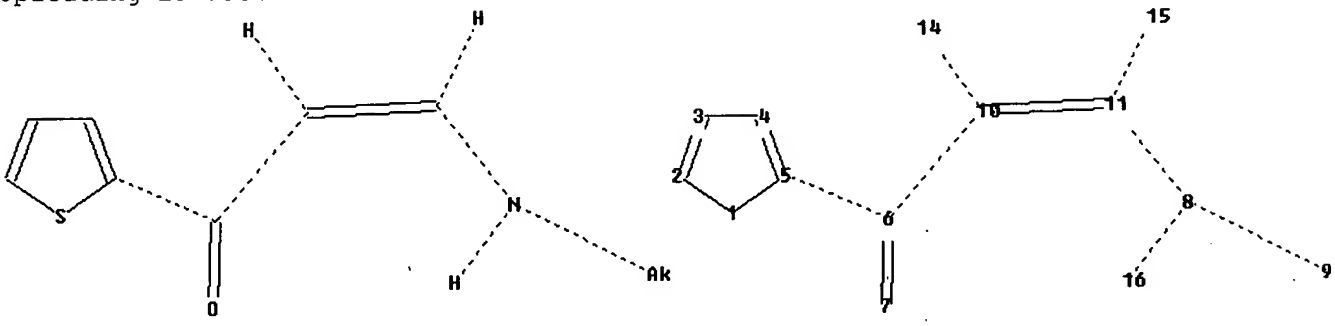
Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom

L7 159 SEA FILE=REGISTRY SUB=L3 SSS FUL L5

L37 STR



Structure attributes must be viewed using STN Express query preparation:
Uploading L37.str



chain nodes :
6 7 8 9 10 11 14 15 16
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 8-16 10-11 10-14 11-15
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 8-16 10-11 10-14 11-15

Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom 14:CLASS 15:CLASS 16:CLASS

L39 9 SEA FILE=REGISTRY SUB=L7 SSS FUL L37
L40 7 SEA FILE=CAPLUS ABB=ON PLU=ON L39

=> s (L21 or L25 or L40) not L77
L81 15 (L21 OR L25 OR L40) NOT L77

=> file beilstein
FILE 'BEILSTEIN' ENTERED AT 17:36:43 ON 04 JAN 2007

FILE LAST UPDATED ON JUNE 16, 2006

FILE COVERS 1771 TO 2006.
*** FILE CONTAINS 9,606,495 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
separate documents and can not be searched together in one query.
Reaction data for BEILSTEIN compounds may be displayed
immediately with the display codes PRE (preparations) and REA
(reactions). A substance answer set retrieved after the search
for a chemical name, a compounds with available reaction
information by combining with PRE/FA, REA/FA or more generally
with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
between a BEILSTEIN compound and belonging reactions. For mo
detailed reaction searches BRNs can be searched as reaction
partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

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****
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* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
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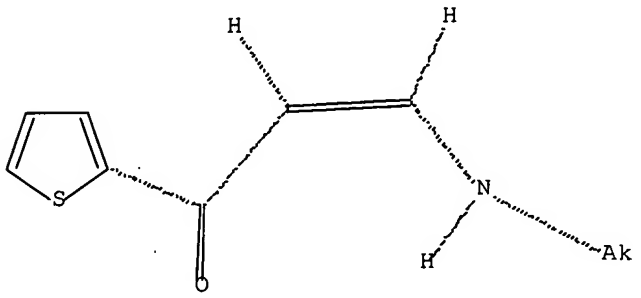
NEW
* *PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.*
* *NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.*

=> d stat que L53
L37 STR



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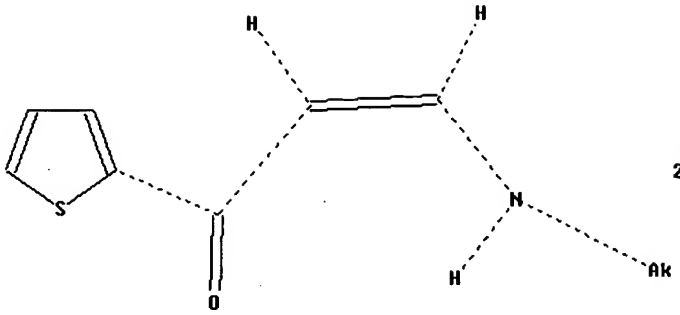

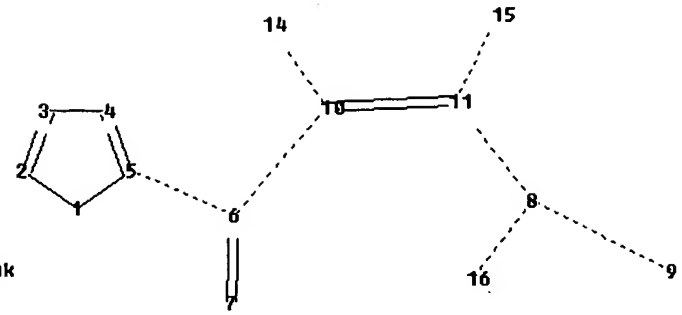

chain nodes :
6 7 8 9 10 11 14 15 16
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 8-16 10-11 10-14 11-15
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 8-16 10-11 10-14 11-15

Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom 14:CLASS 15:CLASS 16:CLASS

L53 1 SEA FILE=BEILSTEIN SSS FUL L37

100.0% PROCESSED 925 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.03

=> file wpix
FILE 'WPIX' ENTERED AT 17:37:01 ON 04 JAN 2007

FILE LAST UPDATED: 2 JAN 2007 <20070102/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200701 <200701/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

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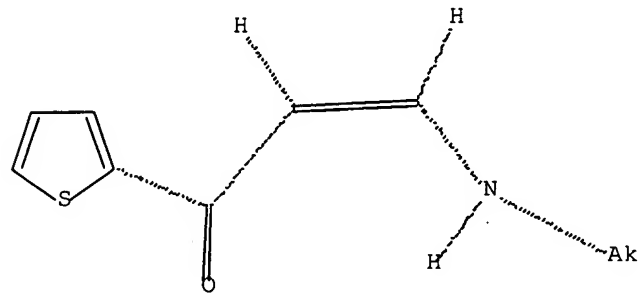
http://www.stn-international.de/stndatabases/details/ipc_reform.html and

http://scientific.thomson.com/media/scpdf/ipcrdwpi.pdf

>>> FOR DETAILS ON THE NEW AND ENHANCED DERWENT WORLD PATENTS INDEX
PLEASE SEE
http://www.stn-international.de/stndatabases/details/dwpi_r.html <<<

'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> d stat que L58
L37 STR



Structure attributes must be viewed using STN Express query preparation:
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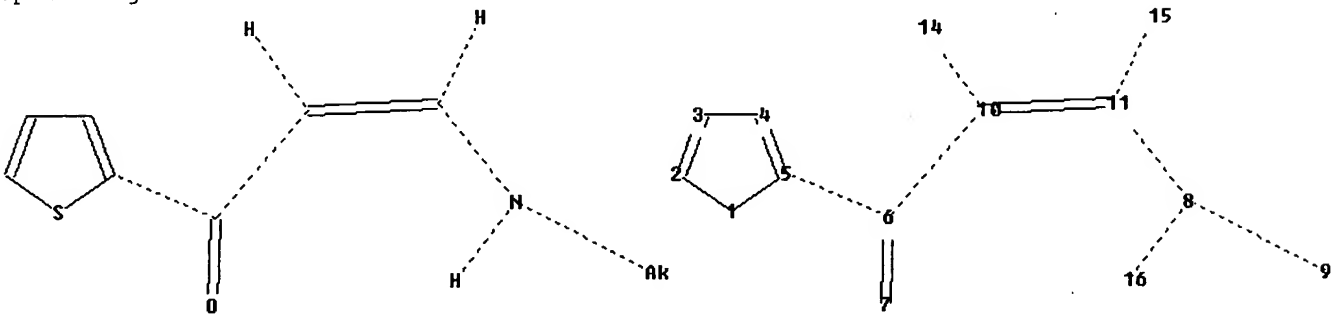

chain nodes :
6 7 8 9 10 11 14 15 16
ring nodes :
1 2 3 4 5
chain bonds :
5-6 6-7 6-10 8-9 8-11 8-16 10-11 10-14 11-15
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 5-6 6-7 6-10 8-9 8-11 8-16 10-11 10-14 11-15

Connectivity :
7:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom
11:Atom 14:CLASS 15:CLASS 16:CLASS

```
L57             1 SEA FILE=WPIX SSS FUL L37
L58             3 SEA FILE=WPIX ABB=ON  PLU=ON  L57/DCR


=> d stat que L59
L59             3 SEA FILE=WPIX ABB=ON  PLU=ON  (RADOK2/DCR,DCN,DRN,DCRE OR
                  873835-0-0-0/DCR,DCN,DRN,DCRE)


=> s (L58 or L59) not L79
L82             2 (L58 OR L59) NOT L79

=> => dup rem L81 L82 L53 L55
DUPLICATE IS NOT AVAILABLE IN 'BEILSTEIN'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
FILE 'CAPLUS' ENTERED AT 17:38:11 ON 04 JAN 2007
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PROCESSING COMPLETED FOR L81
PROCESSING COMPLETED FOR L82
PROCESSING COMPLETED FOR L53
PROCESSING COMPLETED FOR L55
L83            25 DUP REM L81 L82 L53 L55 (3 DUPLICATES REMOVED)
                  ANSWERS '1-15' FROM FILE CAPLUS
                  ANSWER '16' FROM FILE BEILSTEIN
                  ANSWERS '17-25' FROM FILE MARPAT

=> d ibib abs hitind hitstr L83 1-15; d ide allref L83 16; d ibib abs qhit L83 17-
25

L83  ANSWER 1 OF 25  CAPLUS  COPYRIGHT 2007 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2004:1037091  CAPLUS  Full-text
DOCUMENT NUMBER:          142:23180
TITLE:                    Process for producing optically active
                          N-monoalkyl-3-hydroxy-3-arylpropylamine compound and
                          intermediate
INVENTOR(S):              Iwakura, Kazunori; Higashii, Takayuki; Bando, Seiji
PATENT ASSIGNEE(S):       Sumitomo Seika Chemicals Co. Ltd., Japan
SOURCE:                   PCT Int. Appl., 35 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 Japanese
FAMILY ACC. NUM. COUNT:   1
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PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004103990	A1	20041202	WO 2004-JP6602	20040511
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004346008	A	20041209	JP 2003-144742	20030522

PRIORITY APPLN. INFO.: JP 2003-144742 A 20030522

OTHER SOURCE(S): CASREACT 142:23180; MARPAT 142:23180

AB There is provided a process for producing an optically active N-monoalkyl-3-oxo-3-arylpropylamine compound represented by the formula ArC*H(OH)CH2CH2NHR1 (wherein symbol * indicates an asym. carbon atom; R1 represents optionally substituted C1-5 alkyl; Ar represents optionally substituted aryl or heteroaryl) characterized by asym. reducing a (Z)-protected-N-monoalkyl-3-oxo-3-arylpropenylamine compound represented by the formula (Z)-ArCOCH:CHNR1R2 (wherein Ar and R1 are same as defined above; R2 represents an amino-protecting group) with an asym. catalyst to give an optically active compound represented by the formula ArC*H(OH)CH2CH2NR1R2 (wherein the symbol *, Ar, R1, and R2 are same as defined above) and successively eliminating the protective group (R2). Thus, 16.7 g (Z)-N-methyl-3-oxo-3-(2-thienyl)propenylamine was acylated by 16.4 g iso-Bu chlorocarbonate in the presence of 1.2 g 4-dimethylaminopyridine and 12.1 g Et3N in 200 mL tert-Bu Me ether at 50° for 28 h to give 22.0 g N-methyl-N-isobutoxycarbonyl-[(Z)-3-oxo- 3-(2-thienyl)propenyl]amine (I). I (33.8 mg) was stirred in 2-propanol in the presence of potassium tert-butoxide and 2.3 mg [(S)-N-phenyl-2-azetidinecarboxamide]ruthenium(p-cymene) chloride (REG 543689-61-8) at 80° for 4 h to give 84% N-methyl-N-isobutoxycarbonyl-3-hydroxy-3-(2-thienyl)propylamine which (114.8 mg) was treated with a mixture of 0.2 g 30 weight% aqueous NaOH and 5 mL 2-propanol at 30° for 24 h to give N-methyl-3-hydroxy-3-(2-thienyl)propylamine (50% ee).

IC ICM C07D333-20
ICS C07B053-00; C07M007-00

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))

IT Reduction catalysts
(***stereoselective***, ruthenium complexes; preparation of optically active N-monoalkyl-3-hydroxy-3-arylpropylamine compound by asym. reduction of aminovinyl aryl or heteroaryl ketone and deprotection)

IT Reduction
(***stereoselective***; preparation of optically active N-monoalkyl-3-hydroxy-3-arylpropylamine compound by asym. reduction of aminovinyl aryl or heteroaryl ketone and deprotection)

IT 543-27-1, Isobutyl chlorocarbonate ***663603-70-1***, N-Methyl-[(Z)-3-oxo-3-(2-thienyl)propenyl]amine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of optically active N-monoalkyl-3-hydroxy-3-arylpropylamine compound by asym. reduction of aminovinyl aryl or heteroaryl ketone and deprotection)

IT 625853-31-8P, N-Methyl-N-isobutoxycarbonyl-[3-hydroxy-3-(2-thienyl)propyl]amine ***800407-03-8P***, N-Methyl-N-

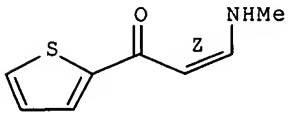
(isobutoxycarbonyl)-[(Z)-3-oxo-3-(2-thienyl)propenyl]amine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active N-monoalkyl-3-hydroxy-3-arylpropylamine compound by asym. reduction of aminovinyl aryl or heteroaryl ketone and deprotection)

IT ***663603-70-1***, N-Methyl-[(Z)-3-oxo-3-(2-thienyl)propenyl]amine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of optically active N-monoalkyl-3-hydroxy-3-arylpropylamine compound by asym. reduction of aminovinyl aryl or heteroaryl ketone and deprotection)

RN 663603-70-1 CAPLUS

CN 2-Propen-1-one, 3-(methylamino)-1-(2-thienyl)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

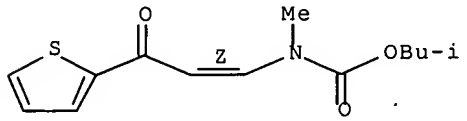


IT ***800407-03-8P***, N-Methyl-N-(isobutoxycarbonyl)-[(Z)-3-oxo-3-(2-thienyl)propenyl]amine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of optically active N-monoalkyl-3-hydroxy-3-arylpropylamine compound by asym. reduction of aminovinyl aryl or heteroaryl ketone and deprotection)

RN 800407-03-8 CAPLUS

CN Carbamic acid, methyl[(1Z)-3-oxo-3-(2-thienyl)-1-propenyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2004:326179 CAPLUS Full-text

DOCUMENT NUMBER: 140:339187

TITLE: Preparation of optically active amino alcohols by asymmetric hydrogenation of enaminones.

INVENTOR(S): Yokozawa, Tohru; Yagi, Kenji; Saito, Takao

PATENT ASSIGNEE(S): Japan

SOURCE: Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

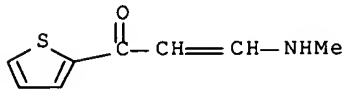
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1411045	A1	20040421	EP 2003-23628	20031016
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004155770	A	20040603	JP 2003-339801	20030930
US 2004082794	A1	20040429	US 2003-686598	20031017
US 6984738	B2	20060110		

PRIORITY APPLN. INFO.: JP 2002-305147 A 20021018
OTHER SOURCE(S): MARPAT 140:339187

AB Optically active R1CH(OH)CHR2CHR3NHR4 [R1 = (substituted) hydrocarbyl, heteroaryl, heterocyclyl; R2, R3 = H, (substituted) hydrocarbyl, acyl, acyloxy, alkoxycarbonyl, aralkoxycarbonyl, aryloxycarbonyl, heteroaryl, heterocyclyl; R4 = H, protecting group; ≥2 of R1-R4 may be bonded to each other to form a ring; with provisos], were prepared by asym. hydrogenation of cis- or trans-R1COCR2:CR3NHR4 (variables as above). Thus, 3-methylamino-1-thiophen-2-ylpropenone, RuCl2[(R)-DM-binap][(R)- daipen] [DM-binap = 2,2'-bis[bis(3,5-dimethylphenyl)phosphino]-1,1'- binaphthyl; daipen = 1,2-di(4-anisyl)-2-isopropyl-1,2-ethylenediamine], and K2CO3 in Me2CHOH were autoclaved under 2.5 MPa H2 at 30° for 18 h to give 79.2% (S)-3-methylamino-1-(2-thienyl)propan-1-ol.

IC ICM C07C213-00
ICS C07D333-20
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 25
IT Hydrogenation catalysts
(***stereoselective***, ruthenium complexes; preparation of optically active amino alcs. by asym. hydrogenation of enaminones)
IT Hydrogenation
(***stereoselective***; preparation of optically active amino alcs. by asym. hydrogenation of enaminones)
IT 877-50-9 ***680193-02-6***
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of optically active amino alcs. by asym. hydrogenation of enaminones)
IT ***680193-02-6***
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of optically active amino alcs. by asym. hydrogenation of enaminones)
RN 680193-02-6 CAPLUS
CN 2-Propen-1-one, 3-(methylamino)-1-(2-thienyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:605439 CAPLUS Full-text

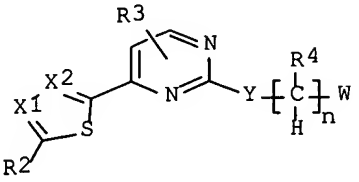
DOCUMENT NUMBER: 145:83372
TITLE: Aminopyrimidine compounds as polo-like kinase 1 inhibitors and their preparation, pharmaceutical compositions and use for treatment of cancer
INVENTOR(S): Smith, Adrian Leonard; Brennan, Paul Edward; Demorin, Frenel Fils; Liu, Gang; Paras, Nick A.; Retz, Daniel Martin
PATENT ASSIGNEE(S): Amgen, Inc., USA
SOURCE: PCT Int. Appl., 151 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006066172	A1	20060622	WO 2005-US45863	20051216

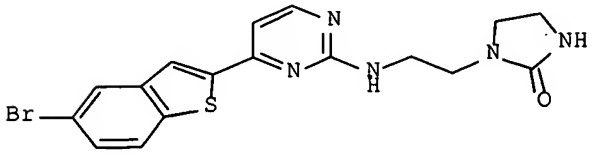
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-636604P P 20041217
OTHER SOURCE(S): MARPAT 145:83372
GI



I



II

AB The invention relates to aminopyrimidine compds. of formula I, which are useful for treating diseases mediated by polo-like kinase 1 (Plk1). The invention also relates to the therapeutic use of such aminopyrimidine compds. and compns. thereof in treating disease states associated with abnormal cell growth and unwanted cell proliferation. Compds. of formula I wherein X1 is

CR1 or N; X2 is CH or N; Y is O, S, CHR7 or NR7; W is CN, (un)substituted imidazolidine, (un)substituted imidazoline, or (un)substituted tetrahydropyrimidine; R1 and R2 are independently H, halo, CN, (un)substituted C1-6 alkyl, (un)substituted alkyl(hetero)aryl, etc.; R3 is H, OH, halo, NO2, NH2, CN, C1-6 alkyl, C1-6 alkoxy, C1-6 alkylamino, C2-6 alkenyl, C2-6 alkynyl, or (hetero)aryl; R4 and R7 are independently H or C1-6 alkyl; n is an integer from 1 to 6; and their pharmaceutically acceptable salts, hydrates and ***stereoisomers*** are claimed. Example compound II was prepared by substitution of 4-(5-bromothien-2-yl)-2- chloropyrimidine with 1-(2-aminoethyl)imidazolidin-2-one. Addnl. 464 example compds. were prepared in this invention. All the invention compds. were evaluated for their human polo-like kinase 1 inhibitory activity. From the assay, it was determined that all the example compds. exhibited plk1 activity with IC50 values less than 1 μM.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT 272-14-0P, Thieno[3,2-c]pyridine 3783-65-1P 4965-26-8P 5713-57-5P 5858-22-0P, 6-Methoxybenzo[b]thiophen-3(2H)-one 6345-55-7P 7465-86-3P, N,N-Diethyl-4-methoxybenzamide 10531-44-9P 13132-15-5P, 2-Benzylthiophene 13196-28-6P 20532-28-9P, Benzo[b]thiophen-5-amine 20699-86-9P 26170-92-3P, 1-(3-Phenylthiophen-2-yl)ethanone 26170-93-4P, 1-(4-Phenylthiophen-2-yl)ethanone 28540-70-7P, 2-Phenethyl-thiophene 34800-30-1P, 2-Bromo-1-(5-iodothiophen-2-yl)ethanone 34843-84-0P, 2-(Thiophen-3-yl)ethanamine hydrochloride 50593-92-5P, 5-Bromo-2-(methylthio)pyrimidine-4-carboxylic acid ***52200-22-3P*** 53442-04-9P 54903-50-3P, 4,5,6,7-Tetrahydro-thieno[3,2-c]pyridine 57275-83-9P, (2-Oxopyrrolidin-1-yl)acetonitrile 58754-96-4P, N-(2,2-Dimethoxyethyl)-4-methyl-N-(thiophen-3-ylmethyl)benzenesulfonamide 58754-97-5P, 2,2-Dimethoxy-N-(thiophen-3-ylmethyl)ethanamine 58754-98-6P, N-(2,2-Dimethoxyethyl)-4-methyl-N-(thiophen-2-ylmethyl)benzenesulfonamide 59906-32-0P 60404-19-5P, 2,3-Dibromo-5-chlorothiophene 66200-61-1P, 1-Phenyl-2-((thiophen-3-ylmethyl)amino)ethanol 66200-62-2P, 7-Phenyl-4,5,6,7-tetrahydro-thieno[3,2-c]pyridine 70298-89-4P, N-(Pyridin-4-yl)pivalamide 71683-02-8P 73120-25-9P 73893-97-7P, 2,2-Dimethoxy-N-(thiophen-2-yl)ethanamine 81597-71-9P 83726-75-4P 87636-27-9P 90407-14-0P, 7-Chlorobenzo[b]thiophene 90407-16-2P, 7-Chlorobenzo[b]thiophene-2-carboxylic acid 90560-10-4P, 6-Methoxybenzo[b]thiophene 91253-06-4P, 1-(Thiophen-2-ylmethyl)piperidine 92885-03-5P, 1-(2-Aminoethyl)pyrrolidin-2-one hydrochloride 105114-80-5P 111881-86-8P, 2-(2-Bromothiophen-3-yl)ethanol 121433-80-5P, 7-Phenyl-4,5-dihydro-thieno[2,3-c]pyridine 129333-20-6P 129333-21-7P 132039-45-3P, 1-(3-(4-Methoxyphenyl)thiophen-2-yl)ethanone ***138716-48-0P*** 160445-19-2P, N-(2-(Thiophen-3-yl)ethyl)benzamide 176214-15-6P, 2-(Methylthio)-5-(trifluoromethyl)pyrimidine 186798-89-0P 209796-22-5P, (2-Bromothiophen-3-yl)acetonitrile 230301-73-2P, tert-Butyl 6,7-dihydro-thieno[3,2-c]pyridine-5(4H)-carboxylate 334971-94-7P, 1-(3-Aminopropyl)imidazolidin-2-one 334971-95-8P, 3-(2-Aminoethyl)-tetrahydro-pyrimidin-2(1H)-one 500366-57-4P 550998-56-6P, Methyl 7-chlorobenzo[b]thiophene-2-carboxylate 596805-19-5P, N,N-Diethyl-4-methoxy-2-(methylthio)benzamide 676448-17-2P, tert-Butyl 4-bromo-1H-indole-1-carboxylate 803603-98-7P 834881-65-1P ***862698-96-2P*** 884603-53-6P 885229-41-4P, 1-(2-Chlorothiazol-5-yl)ethanone 887588-22-9P, 3-(5-Iodothiophen-2-yl)-3-oxopropanenitrile 893421-21-1P 893421-71-1P, 2-(2-Bromothiophen-3-yl)ethanamine 893441-56-0P 893441-57-1P 893441-58-2P ***893441-59-3P*** 893441-60-6P 893441-61-7P 893441-62-8P 893441-63-9P 893441-64-0P 893441-65-1P 893441-66-2P 893441-67-3P 893441-68-4P 893441-69-5P 893441-70-8P 893441-71-9P 893441-72-0P 893441-73-1P 893441-74-2P 893441-75-3P 893441-76-4P 893441-77-5P 893441-78-6P 893441-79-7P 893441-80-0P 893441-81-1P 893441-82-2P

893441-83-3P 893441-84-4P 893441-85-5P 893441-86-6P 893441-87-7P
893441-88-8P 893441-89-9P 893441-90-2P 893441-91-3P 893441-92-4P
893441-94-6P 893441-96-8P 893441-97-9P 893441-98-0P 893441-99-1P
893442-00-7P 893442-01-8P 893442-02-9P ***893442-03-0P***,
3-(Dimethylamino)-1-(3-phenylthiophen-2-yl)prop-2-en-1-one 893442-04-1P,
2-(1,1-Dimethoxyethyl)-3-phenylthiophene 893442-05-2P 893442-06-3P
893442-07-4P 893442-08-5P 893442-09-6P 893442-10-9P 893442-11-0P,
(2-Chlorothiophen-3-yl)acetonitrile 893442-12-1P, 1-(2-(Thiophen-3-
yl)ethyl)pyrrolidine 893442-13-2P 893442-14-3P 893442-15-4P
893442-16-5P 893442-17-6P 893442-18-7P 893442-19-8P 893442-20-1P
893442-21-2P ***893442-22-3P*** 893442-23-4P 893442-24-5P
893442-25-6P 893442-26-7P 893442-27-8P 893442-28-9P
893442-29-0P 893442-30-3P ***893442-31-4P*** 893442-32-5P
893442-33-6P 893442-34-7P 893442-35-8P 893442-36-9P 893442-37-0P
893442-38-1P, 4-(Benzo[b]thiophen-2-yl)-2-(methylthio)-5-
(trifluoromethyl)pyrimidine 893442-39-2P, 4-(Benzo[b]thiophen-2-yl)-5-
(trifluoromethyl)pyrimidin-2-ol 893442-40-5P, 4-(Benzo[b]thiophen-2-yl)-
2-chloro-5-(trifluoromethyl)pyrimidine 893442-41-6P 893442-42-7P
893442-43-8P 893442-44-9P 893442-45-0P 893442-46-1P 893442-47-2P
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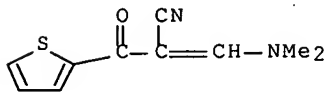
893442-52-9P, 5-(2-Chloroethoxy)benzo[b]thiophene 893442-53-0P
893442-54-1P 893442-55-2P 893442-56-3P 893442-57-4P 893442-58-5P
893442-59-6P 893442-60-9P 893442-61-0P 893442-62-1P 893442-63-2P
893442-64-3P 893442-65-4P 893442-66-5P 893442-67-6P 893442-68-7P
893442-69-8P 893442-70-1P 893442-71-2P 893442-72-3P 893442-73-4P
893442-74-5P, 1-(Thiazol-2-ylmethyl)piperidine 893442-75-6P
893442-76-7P 893442-83-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of aminopyrimidine compds. as polo-like kinase 1 inhibitors and their use for treatment of cancer)

IT ***52200-22-3P 138716-48-0P 862698-96-2P***
893441-59-3P 893442-03-0P, 3-(Dimethylamino)-1-(3-
phenylthiophen-2-yl)prop-2-en-1-one ***893442-22-3P***
893442-25-6P 893442-31-4P 893442-51-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of aminopyrimidine compds. as polo-like kinase 1 inhibitors and their use for treatment of cancer)

RN 52200-22-3 CAPLUS
CN 2-Thiophenepropanenitrile, α-[(dimethylamino)methylene]-β-oxo- (9CI) (CA INDEX NAME)



RN 138716-48-0 CAPLUS
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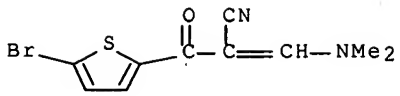
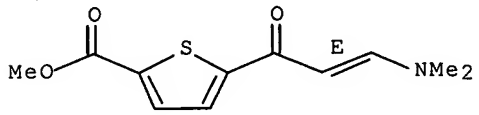


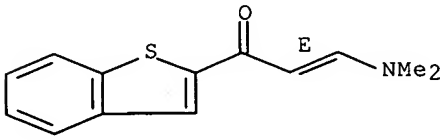
RN 862698-96-2 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-[(2E)-3-(dimethylamino)-1-oxo-2-propenyl]-, methyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

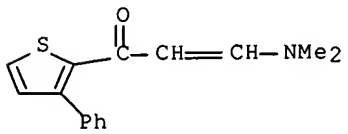


RN 893441-59-3 CAPLUS
CN 2-Propen-1-one, 1-benzo[b]thien-2-yl-3-(dimethylamino)-, (2E)- (9CI) (CA INDEX NAME)

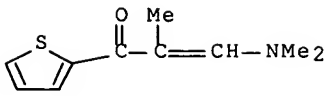
Double bond geometry as shown.



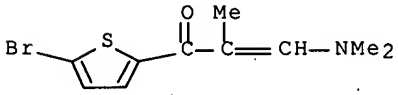
RN 893442-03-0 CAPLUS
CN 2-Propen-1-one, 3-(dimethylamino)-1-(3-phenyl-2-thienyl)- (9CI) (CA INDEX NAME)



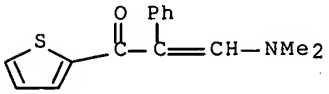
RN 893442-22-3 CAPLUS
CN 2-Propen-1-one, 3-(dimethylamino)-2-methyl-1-(2-thienyl)- (9CI) (CA INDEX NAME)



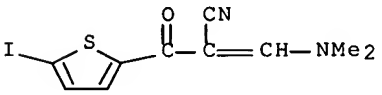
RN 893442-25-6 CAPLUS
CN 2-Propen-1-one, 1-(5-bromo-2-thienyl)-3-(dimethylamino)-2-methyl- (9CI) (CA INDEX NAME)



RN 893442-31-4 CAPLUS
CN 2-Propen-1-one, 3-(dimethylamino)-2-phenyl-1-(2-thienyl)- (9CI) (CA INDEX NAME)



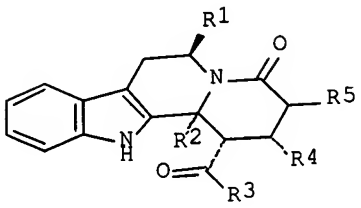
RN 893442-51-8 CAPLUS
CN 2-Thiophenepropanenitrile, α-[(dimethylamino)methylene]-5-iodo-β-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1271087 CAPLUS Full-text
DOCUMENT NUMBER: 144:170909
TITLE: A diversity oriented four-component approach to tetrahydro-β-carbolines initiated by Sonogashira coupling
AUTHOR(S): Karpov, Alexei S.; Rominger, Frank; Mueller, Thomas J. J.
CORPORATE SOURCE: Organisch-Chemisches Institut der Ruprecht-Karls-Universitaet Heidelberg, Heidelberg, D-69120, Germany
SOURCE: Organic & Biomolecular Chemistry (2005), 3(24), 4382-4391

CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:170909
GI



I

AB A consecutive four-component synthesis of highly-substituted tetrahydro-β-carbolines I [R1 = H, MeO2C; R2 = H, n-Bu, Ph, Me3CSiMe2OCH2; R3 = Me2CH, 2-thienyl, 4-O2NC6H4, 4-MeOC6H4, 1-phenylsulfonyl-3-indolyl; R4, R5 = H, Me] can be achieved by a coupling-amination-aza-annulation-Pictet-Spengler (CAAPS) sequence creating five new σ-bonds and four new ***stereocenters*** in a one-pot fashion. The structures were unambiguously supported by X-ray structure analyses.

CC 28-2 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 75

IT Cyclocondensation reaction
(Pictet-Spengler; ***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides)

IT Coupling reaction
(Sonogashira; ***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides)

IT Acid halides
RL: RCT (Reactant); RACT (Reactant or reagent)
(acid chlorides; ***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides)

IT Coupling reaction
(four-component; ***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides)

IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(primary; ***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides)

IT ***Stereoselective*** synthesis

(***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides)

IT Alkynes
RL: RCT (Reactant); RACT (Reactant or reagent)
(α-; ***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides)

IT 725211-48-3P 725211-49-4P 725211-50-7P 725211-52-9P 725211-53-0P
725211-55-2P 874634-26-1P 874634-27-2P 874634-28-3P 874634-29-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides and their crystal structures)

IT 623-47-2, Ethyl propiolate
RL: RCT (Reactant); RACT (Reactant or reagent)
(***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides and their crystal structures)

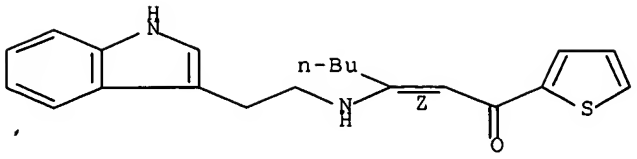
IT ***874634-31-8P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides and their crystal structures)

IT 725211-51-8P 725211-54-1P 725211-56-3P 874634-23-8P 874634-24-9P
874634-25-0P 874634-30-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides and their crystal structures)

IT ***874634-31-8P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(***stereoselective*** preparation of functionalized tetrahydro-β-carbolines by Sonogashira coupling-initiated four-component coupling of aroyl chlorides, α-alkynes, indolyl amines and α,β-unsatd. acyl chlorides and their crystal structures)

RN 874634-31-8 CAPLUS
CN 2-Hepten-1-one, 3-[[2-(1H-indol-3-yl)ethyl]amino]-1-(2-thienyl)-, (2Z)-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



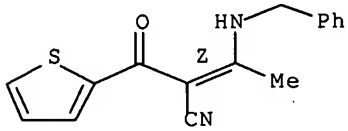
REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 5 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1283908 CAPLUS Full-text
DOCUMENT NUMBER: 144:170660
TITLE: One-pot conversion of β-aminocrotononitrile to secondary enaminonitriles including chiral ones. application to synthesis
AUTHOR(S): Chatterjee, A.; Mishra, M.; Chowdhury, S. K. Dutta; Mahalanabis, Kumar K.
CORPORATE SOURCE: Department of Chemistry, Jadavpur University, Kolkata, 700 032, India
SOURCE: Canadian Journal of Chemistry (2005), 83(8), 1164-1170
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:170660

AB A highly efficient one-pot conversion of β-aminocrotononitrile to secondary enaminonitriles including chiral ones is described. In contrast to β-aminocrotononitrile, some of these N-substituted β-enaminonitriles on reacting with acid chlorides show a unique preference for C-terminal selection allowing preparation of pyrazoles without separation of regioisomers. In addition, use of secondary enaminonitriles also provided access to pyrazoles that are not obtainable with primary enaminonitriles owing to an exclusive preference for N-terminal selection.

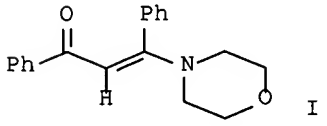
CC 23-19 (Aliphatic Compounds)
IT 874272-55-6P 874272-56-7P 874272-57-8P ***874272-58-9P*** 874272-59-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(acylation of benzylaminocrotononitrile with acid chloride)
IT ***874272-58-9P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(acylation of benzylaminocrotononitrile with acid chloride)
RN 874272-58-9 CAPLUS
CN 2-Thiophenepropanenitrile, β-oxo-α-[1-[(phenylmethyl)amino]ethylidene]-, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

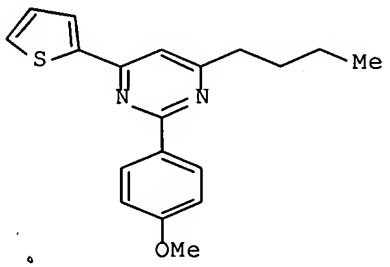


REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:9866 CAPLUS Full-text
DOCUMENT NUMBER: 140:181405
TITLE: Straightforward novel one-pot enaminone and pyrimidine syntheses by coupling-addition-cyclocondensation sequences
AUTHOR(S): Karpov, Alexei S.; Mueller, Thomas J. J.
CORPORATE SOURCE: Organisch-Chemisches Institut der Ruprecht-Karls-Universitaet Heidelberg, Heidelberg, 69120, Germany
SOURCE: Synthesis (2003), (18), 2815-2826
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:181405
GI



I



II

AB One-pot, three-component syntheses of enaminones, e.g., I, and pyrimidines, e.g., II, are reported. The coupling of acid chlorides with terminal alkynes, under modified Sonogashira conditions, followed by addition of primary or secondary amines gave enaminones in excellent yield. 2,4-Di- and 2,4,6-trisubstituted pyrimidines were synthesized, in moderate to good yields, by a one-pot coupling-addition-cyclocondensation sequence of acid chlorides, terminal alkynes and amidine salts.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

IT Acid halides
RL: RCT (Reactant); RACT (Reactant or reagent)
(acid chlorides; ***stereoselective*** preparation of enaminones via Sonogashira coupling of acid chlorides with terminal alkynes followed by ***stereoselective*** conjugate addition of amines)

IT Addition reaction
(conjugate, ***stereoselective***; ***stereoselective*** preparation of enaminones via Sonogashira coupling of acid chlorides with terminal alkynes followed by ***stereoselective*** conjugate addition of amines)

IT Ketones, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(enamino; ***stereoselective*** preparation of enaminones via Sonogashira coupling of acid chlorides with terminal alkynes followed by ***stereoselective*** conjugate addition of amines)

IT Enamines
RL: SPN (Synthetic preparation); PREP (Preparation)
(oxo; ***stereoselective*** preparation of enaminones via Sonogashira coupling of acid chlorides with terminal alkynes followed by ***stereoselective*** conjugate addition of amines)

IT ***Stereoselective*** synthesis
(***stereoselective*** preparation of enaminones via Sonogashira coupling of acid chlorides with terminal alkynes followed by ***stereoselective*** conjugate addition of amines)

IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(***stereoselective*** preparation of enaminones via Sonogashira coupling of acid chlorides with terminal alkynes followed by ***stereoselective*** conjugate addition of amines)

IT Alkynes
RL: RCT (Reactant); RACT (Reactant or reagent)
(α-; ***stereoselective*** preparation of enaminones via Sonogashira coupling of acid chlorides with terminal alkynes followed by ***stereoselective*** conjugate addition of amines)

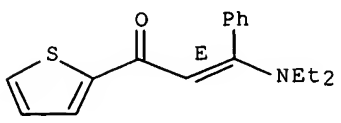
IT 61-54-1, 3-(2-Aminoethyl)indole 98-88-4, Benzoyl chloride 100-46-9, Benzylamine, reactions 109-73-9, 1-Butylamine, reactions 109-89-7, Diethylamine, reactions 110-91-8, Morpholine, reactions 123-75-1, Pyrrolidine, reactions 536-74-3, Phenylacetylene 609-65-4, 2-Chlorobenzoyl chloride 693-02-7, 1-Hexyne 3282-30-2, Pivaloyl chloride 5271-67-0, 2-Thiophenecarboxylic acid chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(***stereoselective*** preparation of enaminones via Sonogashira coupling of acid chlorides with terminal alkynes followed by ***stereoselective*** conjugate addition of amines)

IT 23674-58-0P 70008-81-0P 145799-91-3P 658699-71-9P 658699-72-0P ***658699-73-1P*** 658699-74-2P 658699-75-3P ***658699-76-4P*** ***658699-77-5P*** ***658699-78-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(***stereoselective*** preparation of enaminones via Sonogashira coupling of acid chlorides with terminal alkynes followed by ***stereoselective*** conjugate addition of amines)

IT ***658699-73-1P*** ***658699-76-4P*** ***658699-77-5P*** ***658699-78-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(***stereoselective*** preparation of enaminones via Sonogashira coupling of acid chlorides with terminal alkynes followed by ***stereoselective*** conjugate addition of amines)

RN 658699-73-1 CAPLUS
CN 2-Propen-1-one, 3-(diethylamino)-3-phenyl-1-(2-thienyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 658699-76-4 CAPLUS
CN 2-Propen-1-one, 3-(butylamino)-3-phenyl-1-(2-thienyl)-, (2Z)- (9CI) (CA INDEX NAME)

OTHER SOURCE(S): CASREACT 132:308302
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Transformation of the newly synthesized alkano[c]pyridazines and 1,7-propanothienopyridazines into 1,8-propanophthalazinones and 1,9-propanothiepinopyridazinones using [4+2] cycloaddn. reaction with electron poor olefins and acetylenedicarboxylate derivs., resp. is described. Thus, cyclopentylidenemalononitrile and cyclohexylidenemalononitrile coupled with RN2+.Cl- (R = Ph, 4-O2NC6H4, 4-MeOC6H4, 5-methyl-3-pyrazolyl) to give the cycloalkanopyridazinimines I (n = 1, 2); reaction of I (n = 2, R = Ph; n = 1, R = 5-methyl-3-pyrazolyl) with elemental sulfur gave the corresponding 5,5'-dithiobis(cycloalkanopyridazinones). The propanothienopyridazines II (R1 = Ph, 4-O2NC6H4) were prepared by two methods and underwent cycloaddn. with olefins and acetylenedicarboxylates to give propanophthalazinones III (R2, R3 = EtO2C, EtO2C; NO2, Ph; 2-thienoyl, H; R2R3 = CO-O-CO) and propanothiepinopyridazinones IV (R4 = Me, Et), resp. I reacted with arylidenemalonitriles or a (dimethylamino)propenoylthiophene to give propanophthalazines, e.g. V (R4 = H, MeO, NO2, Cl).

CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))

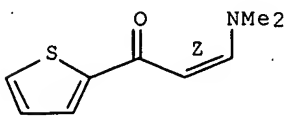
IT 100-05-0, 4-Nitrobenzenediazonium chloride 100-34-5, Benzenediazonium chloride 108-31-6, 2,5-Furandione, reactions 136-35-6 141-05-9, Diethyl maleate 762-21-0, Diethyl acetylenedicarboxylate 762-42-5, Dimethyl acetylenedicarboxylate 1867-38-5, 4-(Chlorobenzylidene)malononitrile 2623-51-0 2700-22-3, Benzylidenemalononitrile 2700-23-4, 4-(Nitrobenzylidene)malononitrile 2826-26-8, 4-(Methoxybenzylidene)malononitrile 4346-59-2, 4-Methoxybenzenediazonium chloride 4354-73-8, Cyclohexylidenemalononitrile 4651-91-6 5660-83-3, Cyclopentylidenemalononitrile 15241-23-3, cis-β-Nitrostyrene 63475-14-9 ***265103-28-4***.
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cycloalkanopyridazinimines, alkanothienopyridazines, and alkanophthalazines via Diels-Alder cycloaddn. reactions)

IT ***265103-28-4***
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cycloalkanopyridazinimines, alkanothienopyridazines, and alkanophthalazines via Diels-Alder cycloaddn. reactions)

RN 265103-28-4 CAPLUS

CN 2-Propen-1-one, 3-(dimethylamino)-1-(2-thienyl)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:445043 CAPLUS Full-text
DOCUMENT NUMBER: 131:184902
TITLE: Reactions of aromatic and heteroaromatic β-amino-β-(polyfluoroalkyl)vinyl ketones with ethylenediamine. A new synthesis of N,N'-unsubstituted imidazolidines
AUTHOR(S): Sosnovskikh, V. Ya.; Kutsenko, V. A.
CORPORATE SOURCE: A. M. Gorky Ural State University, Yekaterinburg, 620083, Russia
SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (1999), 48(3), 540-551
CODEN: RCBUEY; ISSN: 1066-5285
PUBLISHER: Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:184902

AB The reactions of aromatic and heteroarom. β-amino-β- (polyfluoroalkyl)vinyl ketones with ethylenediamine results in the formation of 2,3-dihydro-1H-1,4-diazepines, N,N'-unsubstituted imidazolidines, or N,N'-ethylenebis(aminovinyl ketones). The route depends on the reaction conditions, the nature of the substituent at the carbonyl group, and the number of fluorine atoms in the polyfluoroalkyl radical.

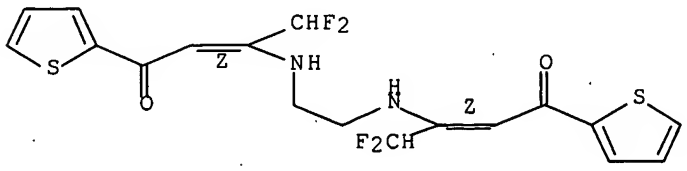
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 77855-08-4P 77855-10-8P 109541-37-9P 109541-38-0P 109541-39-1P
109541-40-4P 139593-54-7P 142968-04-5P 221317-92-6P 221317-94-8P
221317-95-9P 240417-88-3P 240417-89-4P 240417-90-7P 240417-91-8P
240417-92-9P 240417-93-0P 240417-94-1P 240417-95-2P 240417-96-3P
240417-97-4P 240417-98-5P 240417-99-6P 240418-00-2P 240418-01-3P
240418-02-4P 240418-03-5P 240418-05-7P 240418-06-8P 240418-07-9P
240418-08-0P 240418-09-1P 240418-10-4P 240418-11-5P 240418-12-6P
240418-13-7P 240418-14-8P 240418-15-9P ***240418-16-0P***
240418-17-1P 240418-18-2P 240418-19-3P 240418-20-6P 240418-21-7P
240418-22-8P 240418-23-9P ***240418-24-0P*** 240418-25-1P
240418-26-2P ***240418-27-3P*** 240418-28-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT ***240418-16-0P 240418-24-0P 240418-27-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 240418-16-0 CAPLUS
CN 2-Buten-1-one, 3,3'-(1,2-ethanediyldiimino)bis[4,4-difluoro-1-(2-thienyl)-, (2Z,2'Z)- (9CI) (CA INDEX NAME)

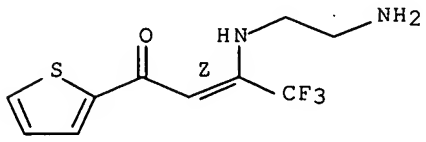
Double bond geometry as shown.



RN 240418-24-0 CAPLUS
CN 2-Buten-1-one, 3-[(2-aminoethyl)amino]-4,4,4-trifluoro-1-(2-thienyl)-,

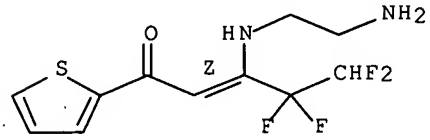
(2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 240418-27-3 CAPLUS
CN 2-Penten-1-one, 3-[(2-aminoethyl)amino]-4,4,5,5-tetrafluoro-1-(2-thienyl)-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 10 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:30401 CAPLUS Full-text
DOCUMENT NUMBER: 120:30401
TITLE: Studies of the π-electron distribution in push-pull alkenes by proton and carbon-13 NMR spectroscopy. II
AUTHOR(S): Kleinpeter, E.; Thomas, S.; Uhlig, G.; Rudorf, W. D.
CORPORATE SOURCE: Fachbereich Chem., Martin-Luther-Univ., Halle/Saale, D(O)-4050, Germany
SOURCE: Magnetic Resonance in Chemistry (1993), 31(8), 714-21
CODEN: MRCHEG; ISSN: 0749-1581
DOCUMENT TYPE: Journal
LANGUAGE: English

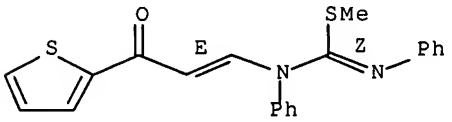
AB A wide variety of push-pull alkenes were studied by means of variable-temperature 1H and 13C NMR spectroscopy with respect to the configuration/conformation and the barriers to rotation about partial C-C and C-N double bonds. For the assignment of the 13C NMR spectra especially the semi-selective INEPT pulse sequence and as incremental system for estimating the 13C chemical shift values of aromatic carbon atoms proved useful. The influence of thioether, sulfone and sulfoxide moieties in the acceptor part of the push-pull system on the π-electron distribution is critically considered.

CC 22-10 (Physical Organic Chemistry)

IT 139427-24-0 139427-25-1 139427-28-4 139427-29-5 139427-31-9
139427-33-1 139427-34-2 145449-38-3 145449-39-4 145449-42-9
151991-19-4 151991-20-7 151991-21-8 151991-22-9 151991-24-1
151991-25-2 151991-26-3 151991-27-4 151991-28-5 151991-29-6
151991-30-9 151991-31-0 151991-32-1 151991-33-2 151991-34-3
151991-35-4 151991-36-5 151991-38-7 151991-39-8 151991-40-1
151991-41-2 151991-42-3 151991-43-4 151991-44-5

151991-45-6 151991-46-7
RL: PRP (Properties)
(NMR of)
IT ***151991-41-2***
RL: PRP (Properties)
(NMR of)
RN 151991-41-2 CAPLUS
CN Carbamimidothioic acid, N-[3-oxo-3-(2-thienyl)-1-propenyl]-N,N'-diphenyl-, methyl ester, (Z,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L83 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:611677 CAPLUS Full-text
DOCUMENT NUMBER: 117:211677
TITLE: Synthesis, chemical, and biological properties of vinylogous hydroxamic acids: dual inhibitors of 5-lipoxygenase and IL-1 biosynthesis
AUTHOR(S): Wright, Stephen W.; Harris, Richard R.; Kerr, Janet S.; Green, Alicia M.; Pinto, Donald J.; Bruin, Elaine M.; Collins, Robert J.; Dorow, Roberta L.; Mantegna, Lisa R.; et al.
CORPORATE SOURCE: Inflammatory Dis. Res., Du Pont Merck Pharm. Co., Wilmington, DE, 19880-0353, USA
SOURCE: Journal of Medicinal Chemistry (1992), 35(22), 4061-8
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:211677
AB Vinylogous hydroxamic acids, 3-(N-hydroxy-N-alkylamino)-2-propen-1-ones (VHAs), were prepared as antiinflammatory agents. The synthesis, chemical properties, and in vitro biol. activities of these relatively unexplored compds. are described. The VHAs were prepared by condensation of the appropriate N-substituted hydroxylamine with any of three reagents: a 1,3-dicarbonyl compound, a vinylogous amide, or an alkynone. The VHAs exist as one or more tautomers in solution with the relative proportions of each being dependent upon the structure of the VHA, solvent, and pH. VHAs undergo some of the typical reactions of hydroxamic acids as well as those of vinylogous amides. VHAs are active as inhibitors of 5-lipoxygenase and of IL-1 biosynthesis in vitro, which do not inhibit other enzymes of the arachidonic acid cascade. They have been shown by ESR studies to bring about inhibition of soybean type 1 15-lipoxygenase by reduction of the active site iron.
CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 1
IT 143620-64-8P 143620-65-9P 143620-67-1P 143620-73-9P 143620-89-7P
143620-90-0P ***143621-01-6P*** 143621-02-7P 143621-03-8P
143621-04-9P 143621-08-3P 143621-09-4P 143621-10-7P 143621-12-9P
143621-13-0P 143621-14-1P 143621-16-3P 143621-17-4P 143621-19-6P
143621-20-9P 143621-21-0P 143621-22-1P 143621-23-2P 143621-24-3P
143621-25-4P 143621-26-5P 143621-30-1P 143631-85-0P 143631-86-1P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and inhibition by, of 5-lipoxygenase and IL-1 biosynthesis)

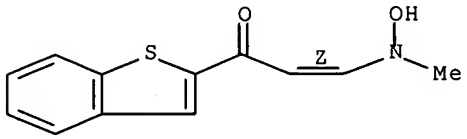
IT 143620-66-0P 143620-68-2P 143620-69-3P 143620-70-6P 143620-71-7P
143620-72-8P 143620-74-0P 143620-75-1P 143620-76-2P 143620-91-1P
143620-92-2P 143620-94-4P 143620-95-5P 143620-96-6P 143620-97-7P
143620-98-8P 143620-99-9P 143621-00-5P 143621-05-0P 143621-06-1P
143621-07-2P 143621-11-8P 143621-15-2P 143621-18-5P 143621-27-6P
143621-28-7P ***143621-29-8P*** 143631-83-8P 143631-87-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and inhibition of 5'-lipoxygenase by)

IT ***143621-01-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and inhibition by, of 5-lipoxygenase and IL-1 biosynthesis)

RN 143621-01-6 CAPLUS

CN 2-Propen-1-one, 1-benzo[b]thien-2-yl-3-(hydroxymethylamino)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

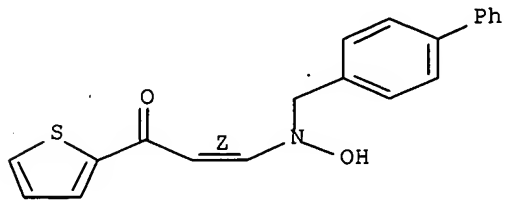


IT ***143621-29-8P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and inhibition of 5'-lipoxygenase by)

RN 143621-29-8 CAPLUS

CN 2-Propen-1-one, 3-[([1,1'-biphenyl]-4-ylmethyl)hydroxyamino]-1-(2-thienyl)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L83 ANSWER 12 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:497263 CAPLUS Full-text

DOCUMENT NUMBER: 95:97263

TITLE: Reaction of β-mercaptoethylamine with α-acetylenic ketones

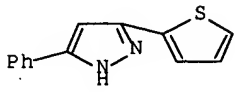
AUTHOR(S): Glotova, T. E.; Nakhmanovich, A. S.; Skvortsova, G. G.; Komarova, T. N.; Kalikhman, I. D.; Voronkov, M. G.

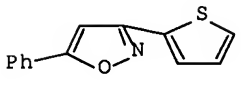
CORPORATE SOURCE: Irkutsk. Inst. Org. Khim., Irkutsk, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1981), 17(4), 749-55
CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 95:97263
GI


IV


V

AB Q = 2-thienyl throughout. Addition reaction of RCOC.tplbond.CR1 (I) (R, R1 = Ph, H; Ph, Ph; Q, H; Q, Ph) with HSCH2CH2NH2 in MeOH-MeONa or CHCl3-K2CO3 gave 8-46% (RCOCH:CR1NHCH2CH2S)2 (II); I (R1 = Ph) also gave 6-56% RCOCH:CPhSCH2CH2NHCPh:CHCOR (III). II formed Cu complexes. Several reactions of III were studied; e.g., with N2H4 or NH2OH, III (R = Q) eliminated HSCH2CH2NH2 to give, resp., IV and V.

CC 25-15 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 27, 28

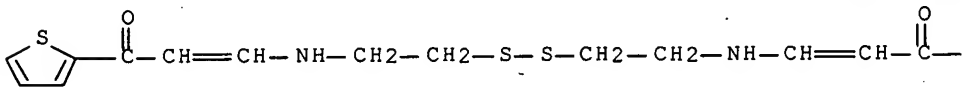
IT 1145-01-3P 2039-49-8P 21985-07-9P 21985-10-4P 78504-82-2P
78504-83-3P ***78504-84-4P*** 78504-85-5P 78504-87-7P
78736-66-0P 78736-67-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT ***78504-84-4P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

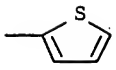
RN 78504-84-4 CAPLUS

CN 2-Propen-1-one, 3,3'-[dithiobis(2,1-ethanediylimino)]bis[1-(2-thienyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



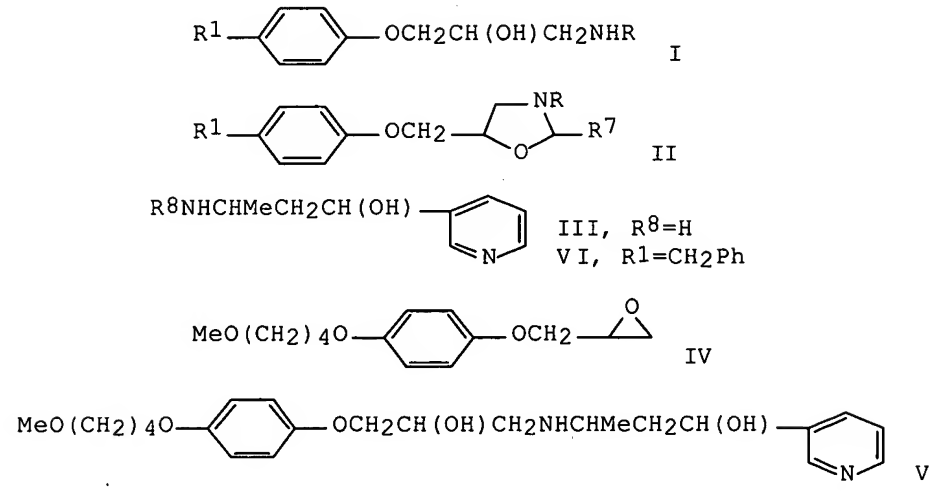
L83 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:105153 CAPLUS Full-text
DOCUMENT NUMBER: 88:105153
TITLE: 1-Phenoxy-3-aminopropan-2-ol derivatives and their acid addition salts
PATENT ASSIGNEE(S): Cassella Farbwerke Mainkur A.-G., Fed. Rep. Ger.
SOURCE: Austrian, 17 pp.

CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 339307	B	19771010	AT 1974-10167	19741219
AT 7410167	A	19770215		
US 4088764	A	19780509	US 1974-531344	19741210
FI 7403631	A	19750628	FI 1974-3631	19741216
NO 7404530	A	19750630	NO 1974-4530	19741216
SE 7415761	A	19750630	SE 1974-15761	19741216
DK 7406547	A	19750825	DK 1974-6547	19741216
DD 117071	A5	19751220	DD 1974-183198	19741219
ZA 7408082	A	19760128	ZA 1974-8082	19741219
SU 559643	A3	19770525	SU 1974-2085461	19741219
SU 598557	A3	19780315	SU 1974-2085234	19741219
HU 171726	B	19780328	HU 1974-CA376	19741219
CA 1047512	A1	19790130	CA 1974-216421	19741219
US 4066768	A	19780103	US 1976-669995	19760324

PRIORITY APPLN. INFO.: LU 1973-34590 A 19731227
US 1974-531344 A2 19741210

GI



AB The title compds. I [R = CR2:CHCOR3, CHR2CH2CH(OH)R3 (R2 = H, Me; R3 = an aromatic or quasi-aromatic 5- or 6-membered monocyclic ring, with 1 or 2 N, O, and (or) S atoms, which can be substituted with 1 or more Me groups, and connected via a C atom); R1 = alkoxymethyl, alkoxyalkoxy, hydroxyalkoxy, NHCONR4R5 (R4 and R5 = H, alkyl, alkenyl, cycloalkyl; NR4R5 = a saturated 5- or 6-membered heterocyclic group, which may have O or S as an addnl. heteroatom), and contain C1-4 alkyl or alkoxy groups, C3-4 alkenyl groups, or C5-7 cycloalkyl groups] as well as their aldehyde condensation products and acid addition salts, were prepared by treating 4-R1C6H4OCH2R6 [R6 = 2-

oxiranyl, CH(OH)CH2X (X = halo) with H2NR (R as above) and the compds. formed, if necessary, converted with R7CHO (R7 = H, C1-4 alkyl) into the oxazolidine II, or, with acid into the acid addition salts. Thus, e.g., aminobutanol III in PhMe was treated with epoxide IV and the mixture stirred 36 h at room temperature to give the dihydroxyamine V. III was prepared by treating nicotinoylacetone K salt in EtOH with PhCH2NH2.HCl, stirring the mixture 24 h at room temperature (88% yield), reducing the product R9CH:CMeNHCH2Ph (R9 = nicotinoyl) with NaBH4 (62% yield), and debenzylating the amino alc. VI. An addnl. 57 I and 1 oxazolidine derivative were prepared Selected I had ED50 0.003-0.093 mg/kg (dog) as β1-receptor inhibitors and ED50 1.02-15.59 mg/kg (dog) as β2-receptor inhibitors [vs. 0.238 and 26.505 for 4-Me2CHNHCH2CH(OH)CH2OC6H4NHAc] and are useful in treating arrhythmia and other heart disorders.

IC C07D213-30

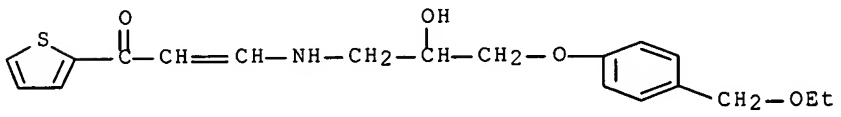
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 28

IT 57725-38-9P 57725-46-9P 57725-47-0P 57725-48-1P ***57725-49-2P***
57725-50-5P 57725-51-6P 57725-53-8P 57725-54-9P 57725-55-0P
57725-56-1P 57725-57-2P 57725-58-3P 57725-60-7P 57725-61-8P
57725-62-9P 57725-63-0P 57725-65-2P 57725-66-3P 57725-67-4P
57725-68-5P 57725-69-6P 57725-70-9P 57725-71-0P 57725-72-1P
57725-73-2P 57725-74-3P 57725-75-4P 57725-76-5P 57725-77-6P
57725-78-7P 57725-79-8P 57725-80-1P 57725-81-2P 57725-82-3P
57725-83-4P 57725-84-5P 57725-85-6P 57725-86-7P 57725-87-8P
57725-88-9P 57725-89-0P 57725-90-3P 57725-91-4P 57725-92-5P
57725-93-6P 57725-94-7P 57725-95-8P 57726-22-4P 57953-56-7P
57953-58-9P 57953-59-0P 65653-26-1P 65653-37-4P 65653-38-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT ***57725-49-2P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 57725-49-2 CAPLUS

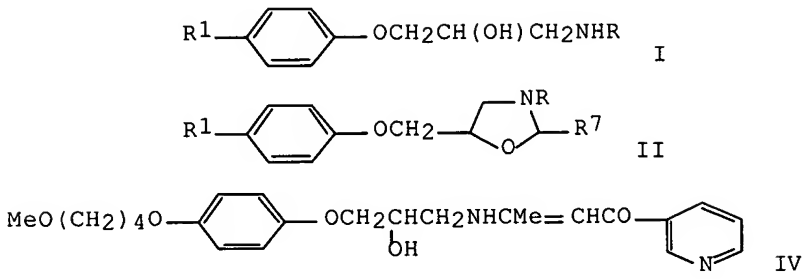
CN 2-Propen-1-one, 3-[[3-[4-(ethoxymethyl)phenoxy]-2-hydroxypropyl]amino]-1-(2-thienyl)- (9CI) (CA INDEX NAME)



L83 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:89525 CAPLUS Full-text
DOCUMENT NUMBER: 88:89525
TITLE: 1-Phenoxy-3-aminopropan-2-ol derivatives and their acid addition salts
PATENT ASSIGNEE(S): Cassella Farbwerke Mainkur A.-G., Fed. Rep. Ger.
SOURCE: Austrian, 20 pp.
CODEN: AUXXAK
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AT 339306	B	19771010	AT 1974-10166	19741219
AT 7410166	A	19770215		
US 4088764	A	19780509	US 1974-531344	19741210
FI 7403631	A	19750628	FI 1974-3631	19741216
NO 7404530	A	19750630	NO 1974-4530	19741216
SE 7415761	A	19750630	SE 1974-15761	19741216
DK 7406547	A	19750825	DK 1974-6547	19741216
DD 117071	A5	19751220	DD 1974-183198	19741219
ZA 7408082	A	19760128	ZA 1974-8082	19741219
SU 559643	A3	19770525	SU 1974-2085461	19741219
SU 598557	A3	19780315	SU 1974-2085234	19741219
HU 171726	B	19780328	HU 1974-CA376	19741219
CA 1047512	A1	19790130	CA 1974-216421	19741219
US 4066768	A	19780103	US 1976-669995	19760324
PRIORITY APPLN. INFO.:			LU 1973-34590 A	19731227
			US 1974-531344 A2	19741210

GI



AB The title compds. I [R = CR2:CHCOR3, CHR2CH2CH(OH)R3 (R2 = H, Me; R3 = an aromatic or quasi-aromatic 5- or 6-membered monocyclic ring, with 1 or 2 N, O, and (or) S atoms, which can be substituted with 1 or more Me groups, and connected via a C atom); R1 = alkoxymethyl, alkoxyalkoxy, hydroxyalkoxy, NHCONR4R5 (R4 and R5 = Ph, alkyl, alkenyl, cycloalkyl; NR4R5 = a saturated 5- or 6-membered heterocyclic group, which may have O or S as an addnl. heteroatom), and contain C1-4 alkyl or alkoxy groups, C3-4 alkenyl groups, and C5-7 cycloalkyl groups] as well as their aldehyde condensation products and acid addition salts, were prepared by treating 4-R1C6H4OCH2CH(OH)CH2NH2 with RR6 (R as above, R6 = halo, OH, OK, ONa) and the obtained I, if necessary, converted with R7CHO (R7 = H, C1-4 alkyl) into oxazolidines II or with an acid into acid addition salts. Thus, e.g., 4-MeO(CH2)4OC6H4OCH2CH(OH)CH2NH2 (III) in EtOH was treated with nicotinoylacetone and the mixture treated with 1 drop HCO2H and refluxed 3 h to give 78% the nicotinoylvinylamino ether IV. Nicotinoylacetone was prepared by dropwise treatment of KOCMe3 in C6H6 with EtOAc and 3-acetylpyridine at 10° and keeping the mixture 24 h at room temperature III was prepared by heating 4-HOC6H4OCH2Ph with MeO(CH2)4Br in Me2CO with excess K2CO3, hydrogenolysis of the formed 4-MeOC6H4OR8 (V, R8 = CH2Ph), treating the phenol V (R = H) with epichlorohydrin, and ammonolysis of the resulting glycidyl ether V (R = glycidyl). An addnl. 54 I and 1 oxazolidine derivative were prepared Selected I had ED50 0.003-0.093 mg/kg (dog) as β1-receptor inhibitors and ED50 1.02-15.59 mg/kg (dog) as β2-receptor inhibitors [vs. 0.238 and 26.505 for 4- Me2CHNHCH2CH(OH)CH2OC6H4NHAc] and are useful in treating arrhythmia and other heart disorders.

IC C07D213-30
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 28
IT 57725-38-9P 57725-45-8P 57725-47-0P 57725-48-1P ***57725-49-2P***
57725-50-5P 57725-51-6P 57725-54-9P 57725-55-0P 57725-56-1P
57725-57-2P 57725-58-3P 57725-59-4P 57725-60-7P 57725-61-8P
57725-62-9P 57725-63-0P 57725-65-2P 57725-66-3P 57725-67-4P
57725-68-5P 57725-69-6P 57725-70-9P 57725-71-0P 57725-72-1P
57725-73-2P 57725-74-3P 57725-75-4P 57725-76-5P 57725-77-6P
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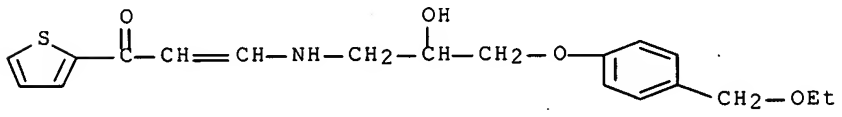
57725-83-4P 57725-84-5P 57725-85-6P 57725-86-7P 57725-87-8P
57725-88-9P 57725-89-0P 57725-90-3P 57725-91-4P 57725-92-5P
57725-93-6P 57725-94-7P 57725-95-8P 57726-22-4P 57953-56-7P
57953-58-9P 57953-59-0P 65653-37-4P 65653-38-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT ***57725-49-2P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 57725-49-2 CAPLUS
CN 2-Propen-1-one, 3-[[3-[4-(ethoxymethyl)phenoxy]-2-hydroxypropyl]amino]-1-(2-thienyl)- (9CI) (CA INDEX NAME)



L83 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:30897 CAPLUS Full-text
DOCUMENT NUMBER: 84:30897
TITLE: Heterocyclic derivatives of 1-amino-3-phenoxy-2-propanol
INVENTOR(S): Raabe, Thomas; Graewinger, Otto; Scholtholt, Josef; Nitz, Rolf E.; Schraven, Eckhard
PATENT ASSIGNEE(S): Cassella Farbwerke Mainkur A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 61 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2458744	A1	19750710	DE 1974-2458744	19741212
NL 7416377	A	19750701	NL 1974-16377	19741216
FR 2255893	A1	19750725	FR 1974-42024	19741219
AU 7476664	A	19760624	AU 1974-76664	19741219
GB 1443135	A	19760721	GB 1974-54911	19741219
ES 433131	A1	19770216	ES 1974-433131	19741219
ES 433132	A1	19770216	ES 1974-433132	19741219
ES 433133	A1	19770216	ES 1974-433133	19741219
CH 602716	A5	19780731	CH 1974-16973	19741219
CH 603584	A5	19780831	CH 1974-16972	19741219

CS 184837	B2	19780915	CS 1974-8779		19741219
CS 184838	B2	19780915	CS 1974-8780		19741219
CS 184850	B2	19780915	CS 1977-1030		19741219
CH 605758	A5	19781013	CH 1974-16974		19741219
RO 69155	A1	19810330	RO 1974-80875		19741219
RO 68397	A1	19810626	RO 1974-80874		19741219
RO 69154	A1	19810730	RO 1974-80873		19741219
JP 50096562	A	19750731	JP 1974-148532		19741226

PRIORITY APPLN. INFO.: LU 1973-69079 A 19731227

AB 1-Phenoxy-3-amino-2-propanols 4-RC6H4OCH2CH(OH)CH2NHR1 (I; R = alkoxymethyl, alkoxyalkoxy, hydroxyalkoxy, or substituted ureido; R1 = CR2:CHCOR3 or CHR2CH2CHR3OH, where R2 = H or Me, and R3 = a C-bonded 5- or 6-membered heterocyclic ring containing 1 or 2 N, S, and/or O atoms), which were β-receptor blocking agents, were prepared by reacting 4-RC6H4OCH2CH(OH)CH2NH2 with R1X, where X = Br or Cl. Among 56 I thus prepared were (R, R1 given): MeO(CH2)4O, CMe:CHCOR3 (R3 = 3-pyridyl); EtOCH2, 2-(2-thienylcarbonyl)vinyl; EtNHCONH, 2-[(2,4-dimethyl-2- pyrimidinyl)carbonyl]-1-methylvinyl; HOCH2CH2O, 3-(1,5-dimethylpyrazol-4- yl)-3-hydroxy-1-methylpropyl; and morpholinocarboxamido, 3-hydroxy-1-methyl-3-(6-methyl-3-pyridyl)propyl.

IC C07D

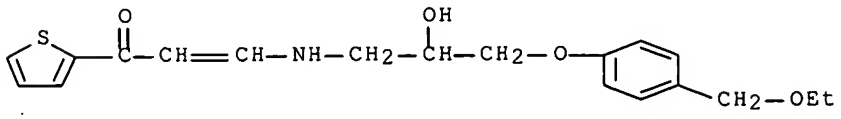
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 25, 28

IT 3051-27-2P 3594-37-4P 18394-65-5P 51469-80-8P 51469-83-1P
56703-83-4P 56704-26-8P 56735-78-5P 57725-38-9P 57725-42-5P
57725-44-7P 57725-45-8P 57725-46-9P 57725-47-0P 57725-48-1P
57725-49-2P 57725-50-5P 57725-51-6P 57725-52-7P
57725-53-8P 57725-54-9P 57725-55-0P 57725-56-1P 57725-57-2P
57725-58-3P 57725-59-4P 57725-60-7P 57725-61-8P 57725-62-9P
57725-63-0P 57725-64-1P 57725-65-2P 57725-66-3P 57725-67-4P
57725-68-5P 57725-69-6P 57725-70-9P 57725-71-0P 57725-72-1P
57725-73-2P 57725-74-3P 57725-75-4P 57725-76-5P 57725-77-6P
57725-78-7P 57725-79-8P 57725-80-1P 57725-81-2P 57725-82-3P
57725-83-4P 57725-84-5P 57725-85-6P 57725-86-7P 57725-87-8P
57725-88-9P 57725-89-0P 57725-90-3P 57725-91-4P 57725-92-5P
57725-93-6P 57725-94-7P 57725-95-8P 57725-96-9P 57725-97-0P
57725-98-1P 57725-99-2P 57726-00-8P 57726-01-9P 57726-02-0P
57726-22-4P 57953-56-7P 57953-57-8P 57953-58-9P 57953-59-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT ***57725-49-2P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

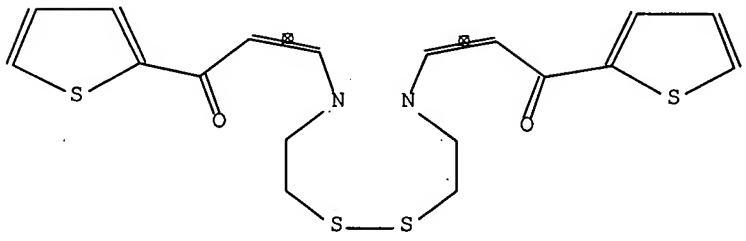
RN 57725-49-2 CAPLUS

CN 2-Propen-1-one, 3-[[3-[4-(ethoxymethyl)phenoxy]-2-hydroxypropyl]amino]-1-(2-thienyl)- (9CI) (CA INDEX NAME)



L83 ANSWER 16 OF 25 BEILSTEIN COPYRIGHT 2007 BEILSTEIN MDL on STN

Beilstein Records (BRN):	5127583
Beilstein Pref. RN (BPR):	78504-84-4
CAS Reg. No. (RN):	78504-84-4
Chemical Name (CN):	bis<6-(2-thienyl)-6-oxo-3-aza-4-hexenyl> disulfide
Autonom Name (AUN):	3-<2-<2-(3-oxo-3-thiophen-2-yl-propenylamino)-ethyldisulfanyl>-ethylamino>-1-thiophen-2-yl-propenone
Molec. Formula (MF):	C18 H20 N2 O2 S4
Molecular Weight (MW):	424.61
Lawson Number (LN):	20597, 3125
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	4556962
Tautomer ID (TAUTID):	4920871
Beilstein Citation (BSO):	6-18
Entry Date (DED):	1992/08/28
Update Date (DUPD):	1993/04/29



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
IR	Infrared Spectrum	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

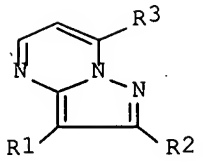
All References:
ALLREF

1. Glotova, T. E.; Nakhmanovich, A. S.; Skvortsova, G. G.; Komarova, T. N.; Kalikhman, I. D.; Voronkov, M. G., J.Org.Chem.USSR (Engl.Transl.), CODEN: JOCYA9, 17(4), <1981>, 653-658, Zh.Org.Khim., CODEN: ZORKAE, 17(4), <1981>, 749-755; BABS-5634488

L83 ANSWER 17 OF 25 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 143:194019 MARPAT Full-text
TITLE: Two-phase method for the synthesis of pyrazolopyrimidine derivatives via heterocyclization of aminopyrazoles with propenone derivatives
INVENTOR(S): Cantrell, Gary Lee; Moser, Frank William; Halvachs, Robert Edward
PATENT ASSIGNEE(S): Mallinckrodt Inc., USA
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005070931	A1	20050804	WO 2004-US40241	20041202
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004314335	A1	20050804	AU 2004-314335	20041202
CA 2553465	A1	20050804	CA 2004-2553465	20041202
EP 1713808	A1	20061025	EP 2004-812693	20041202
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
PRIORITY APPLN. INFO.:			US 2004-536302P	20040114
			WO 2004-US40241	20041202

GI



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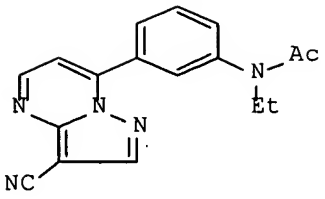
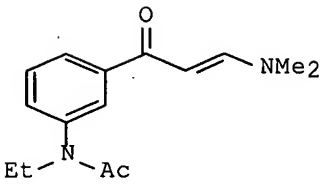


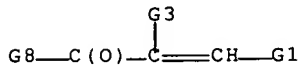
II



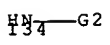
III

AB The invention relates to a two-phase method for the synthesis of pyrazolopyrimidine derivs. of formula I [wherein: R1 is H, F, Cl, formyl, carboxyl, or CN, etc.; R2 is H, F, CN, cyanomethyl, or carbamoyl, etc.; R3 is Ph, o-trifluoromethylphenyl, m-methoxyphenyl, or pyridyl, etc.], useful as anxiolytics, anticonvulsants, or muscle relaxants, etc. (no data). The invention compds. were prepared via heterocyclization of aminopyrazole derivs. or a salt thereof with 1-oxo-2-propenyl-arene(heterocycle) under acidic conditions in a reaction medium including a two-phase mixture of an aqueous solution and a water-immiscible organic liquid For instance, pyrazolopyrimidine derivative II (zaleplon) was prepared via heterocyclization of N-[(oxopropenyl)phenyl]-N-ethylacetamide III with 3-amino-4- cyanopyrazole in 2-phase mixture consisting of water, 2-butanone, and heptafluorobutyric acid with a yield of 100%.

MSTR 3



G1 = 134



G2 = alkyl <containing 1-6 C>
G8 = thienyl
Patent location: claim 15

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 18 OF 25 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 140:199199 MARPAT Full-text

TITLE: Process for preparation of N-monoalkyl-3-hydroxy-3-(2-thienyl)propanamines

INVENTOR(S): Kogami, Kenji; Hayashizaka, Noriyuki; Satake, Syuzo; Fuseya, Ichiro; Kagano, Hirokazu

PATENT ASSIGNEE(S): Sumitomo Seika Chemicals Co., Ltd., Japan

SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004016603	A1	20040226	WO 2003-JP8950	20030715
W: CA, CN, JP, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2493776	A1	20040226	CA 2003-2493776	20030715
EP 1541569	A1	20050615	EP 2003-741391	20030715
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, SK				
CN 1671686	A	20050921	CN 2003-818466	20030715
US 2005240030	A1	20051027	US 2005-523287	20050203
PRIORITY APPLN. INFO.:			JP 2002-229204	20020806
			WO 2003-JP8950	20030715

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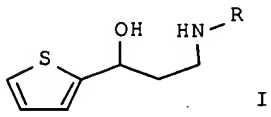
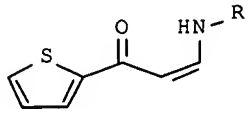


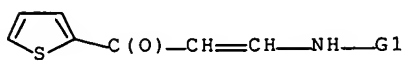
I



II

AB This invention pertains to a method for producing N-monoalkyl-3-hydroxy-3- (2-thienyl)propanamines with general formula of I [where R = alkyl], which comprises reduction of II with NaBH4 or Na(CN)H3. For example, β-oxo-β-(2-thienyl)propanal sodium salt was treated with MeNH2 in MeOH, followed by the addition of aqueous NaOH to give (Z)-N-methyl-3-oxo-3-(2- thienyl)-1-propenamine (74.8%). The propenamine was treated with NaBH4 in PhMe in the presence of AcOH to afford the title compound N-methyl-3-hydroxy-3-(2-thienyl)-1-propanamine (75.0%). By the process, an N-monoalkyl-3-hydroxy-3-(2-thienyl)propanamine useful as an intermediate for various medicines can be industrially and easily produced at low cost.

MSTR 1



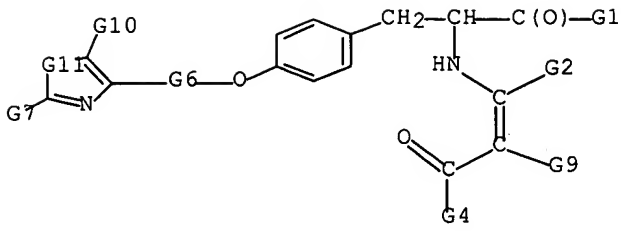
G1 = alkyl <containing 1-4 C>
Patent location: claim 1

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 19 OF 25 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 136:336180 MARPAT Full-text
TITLE: Diabetes diagnosis by genotyping insulin receptor gene single-nucleotide polymorphisms
INVENTOR(S): Hosford, David; Purvis, Ian James
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002033121	A2	20020425	WO 2001-GB4660	20011019
WO 2002033121	A3	20031016		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001095752	A5	20020429	AU 2001-95752	20011019
PRIORITY APPLN. INFO.:			GB 2000-25678	20001019
			WO 2001-GB4660	20011019

AB The invention provides a method of diagnosing diabetes or susceptibility to diabetes in an individual, comprising typing (i) the insulin receptor gene region or (ii) the insulin receptor protein of the individual. The invention also provides a diagnostic kit that comprises a polynucleotide, probe, primer, antibody (including an antibody fragment) or agent as defined herein. The invention also provides a nonhuman animal which has diabetes (typically type II diabetes) or is susceptible to diabetes and which is also transgenic for a polymorphism as mentioned above. The invention provides a method for treating a patient who has been diagnosed as having or being susceptible to diabetes by a method of the invention, comprising administering an effective amount of an anti-diabetes agent or an agent that prevents the development of diabetes to the patient. The inventors have shown that naturally occurring polymorphisms in the insulin receptor are functional. These functional polymorphisms are associated with migraine, a condition that is overrepresented in diabetics. The inventors isolated 48 single-nucleotide polymorphisms within the locus, of which we genotyped in a Caucasian population comprising 827 unrelated cases and 765 controls. Five single-nucleotide polymorphisms within the insulin receptor gene showed significant association with migraine. This association was independently replicated in a case-control population collected sep.

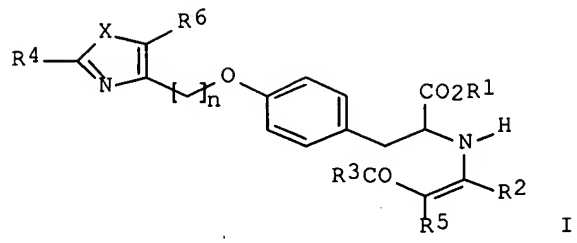


G4 = thienyl
Patent location: claim 15

L83 ANSWER 20 OF 25 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 132:151814 MARPAT Full-text
TITLE: Preparation of substituted oxazoles and thiazoles as hPPAR gamma and hPPAR alpha activators
INVENTOR(S): Collins, Jon Loren; Dezube, Milana; Oplinger, Jeffrey Alan; Willson, Timothy Mark
PATENT ASSIGNEE(S): Glaxo Group Limited, UK
SOURCE: PCT Int. Appl., 110 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000008002	A1	20000217	WO 1999-EP5666	19990805
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2339773	A1	20000217	CA 1999-2339773	19990805
AU 9957310	A1	20000228	AU 1999-57310	19990805
EP 1102757	A1	20010530	EP 1999-944335	19990805
EP 1102757	B1	20040414		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200100372	T2	20010921	TR 2001-20010037219990805	
BR 9912866	A	20011030	BR 1999-12866	19990805
HU 200103469	A2	20020128	HU 2001-3469	19990805
EE 200100074	A	20020617	EE 2001-74	19990805
AT 264313	T	20040415	AT 1999-944335	19990805
ES 2220110	T3	20041201	ES 1999-944335	19990805
ZA 2001000983	A	20020305	ZA 2001-983	20010205
NO 2001000628	A	20010406	NO 2001-628	20010206
HR 2001000095	A1	20020228	HR 2001-95	20010207
US 6498174	B1	20021224	US 2001-762445	20010222
PRIORITY APPLN. INFO.:			GB 1998-17118	19980807
			WO 1999-EP5666	19990805

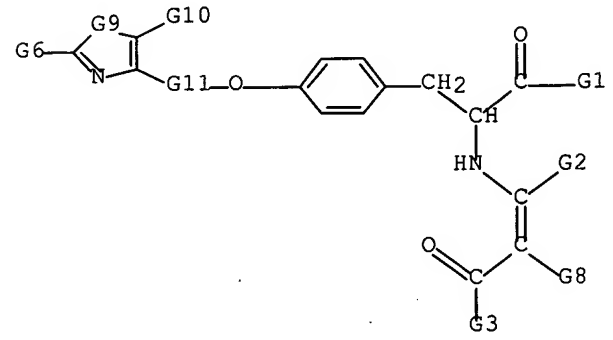
GI



I

AB The title compds. [I; R1 = H, alkyl; R2 = H, alkyl, haloalkyl; R3 = alkyl, cycloalkyl, cycloalkenyl, etc.; R4 = (un)substituted 5-6 membered heterocyclyl containing at least one O, N or S atom, Ph; R5 = H, halo, alkyl, haloalkyl; R6 = H, alkyl; X = O, S; n = 1-3], which are dual activators of hPPARγ and hPPARα, were prepared Thus, refluxing a suspension of (2S)-2-amino-3-{4-[2-(5-methyl-2-phenyl-1,3-oxazol-4- yl)ethoxy]phenyl}propanoic acid (preparation given) and benzoylacetone in MeOH and trimethylorthoformate afforded 43% (2S)-(Z)-I [R1 = H; R2 = Me; R3 = Ph; R4 = Ph; R5 = H; R6 = Me; X = O; n = 2] which showed 39% glucose reduction in rats.

MSTR 1



G3 = thienyl (opt. substd. by 1 or more G12)
Derivative: or tautomers, pharmaceutically acceptable salts, or solvates
Patent location: claim 1

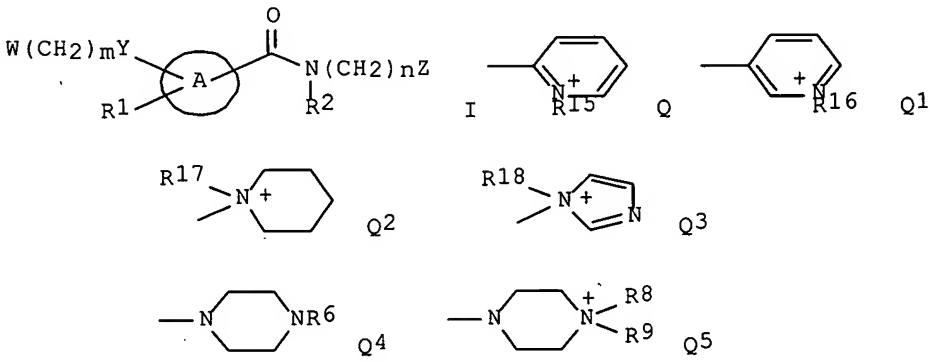
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 21 OF 25 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 130:291600 MARPAT Full-text
TITLE: Amides, bone formation promoters containing them, and their use as antiosteoporotic agents
INVENTOR(S): Shibata, Saizo; Omori, Fujimi; Nakagawa, Takashi

PATENT ASSIGNEE(S): Japan Tobacco, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 45 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11080107	A	19990326	JP 1997-251360	19970901

PRIORITY APPLN. INFO.: JP 1997-251360 19970901
GI



AB Bone formation promoters contain amides I [W = H, amino, NHCOR3 (R3 = lower alkyl), lower alkoxycarbonyl, cycloalkyl, naphthyl, morpholino, thienyl, phthalimido, benzoyl, benzyloxy, C6H4R4 (R4 = H, halo, lower alkyl, lower alkoxy); Y = O, NHCO2, NHCO, CONH, CO, CO2, OCO, CO(CH:CH)u (u = 1, 2), direct bond; ring A = benzene, naphthalene, cyclohexane, biphenyl, di-Ph ether, pyridine, isoxazole, thiophene; R1 = H, halo, NO2, lower alkyl, lower alkoxy; R2 = H, lower alkyl; Z = halo, OH, lower alkyl, lower alkoxy, lower alkoxycarbonyl, carboxy, NR5R6 [R5, R6 = H, (hydroxy)alkyl, aryl, lower alkylcarbonyl], N+R7R8R9 [R7, R8 = lower alkyl, aralkyl; R9 = lower alkyl, (halo)aralkyl, arylcarbonylalkyl], SR10 (R10 = lower alkyl, aralkyl), SO2R11 (R11 = lower alkyl, aralkyl), SOR12 (R12 = lower alkyl, aralkyl), S+R13R14 (R13, R14 = lower alkyl), morpholino, pyridyl, pyridinio, Q (R15 = lower alkyl), Q1 (R16 = lower alkyl), Q2 (R17 = lower alkyl), Q3 (R18 = lower alkyl); R2 and R5 may be bonded to each other to form Q4 (R6 = any group given above); R2 and R7 may be bonded to each other to form Q5 (R8, R9 = any group given above), m = 0-20; n = 0-4] or their pharmaceutically acceptable salts as active ingredients. Pharmaceutical compns. and antiosteoporotic agents containing I or their salts are also claimed. N-[2-(dimethylamino)ethyl]4-(nonyloxy)benzamide hydrochloride (preparation given) at 3 μM showed 244% osteoblast growth promoting activity.

MSTR 1

G1—G17—C(O)—G38
1 2 3

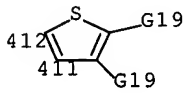
G1 = 11

G8—G6
11 12

G6 = alkylcarbonylamino <containing 1-6 C>
G8 = 25-2 26-12

C(O)G10
25 26

G10 = (1-2) CH=CH
G17 = 412-1 411-3



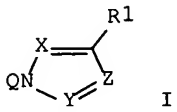
Patent location: claim 1
Note: substitution is restricted

L83 ANSWER 22 OF 25 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 125:195641 MARPAT Full-text
TITLE: Preparation of 5-member heteroaromatic compounds useful as dopamine receptor-subtype ligands
INVENTOR(S): Carling, William Robert; Leeson, Paul David; Moore, Kevin William
PATENT ASSIGNEE(S): Merck Sharp and Dohme Limited, UK
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9621660	A1	19960718	WO 1996-GB6	19960103
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN				
AU 9643123	A	19960731	AU 1996-43123	19960103

US 5939436	A	19990817	US 1997-875059	19970625
PRIORITY APPLN. INFO.:			GB 1995-580	19950112
			WO 1996-GB6	19960103
			WO 1997-EP678	19970213

GI

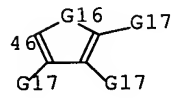


I

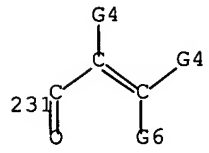
AB The title compds. [I; Q = substituted 5-7-member monocyclic heteroaliph. ring; R1 = (un)substituted Ph, (un)substituted pyridyl, (un)substituted furyl, etc.; X = N, CR1; Y:Z = N:CR1, N:N, HC:N], which are ligands for dopamine receptor subtypes (e.g., D4; I demonstrate a Ki against the binding of [3H]-spiperone to cloned human D4 dopamine receptor of <1.5 μM) and are useful in the treatment and/or prevention of schizophrenia (no data) and depression (no data), are prepared Thus, 1-benzyl-4-[(5- methyl-4-phenyl)pyrazol-1-yl]piperidine dihydrochloride, m.p. 198-201°, was prepared from 4-hydroxypiperidine in 5 steps.

MSTR 4

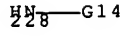
G1 = 46



G2 = 231



G6 = 228



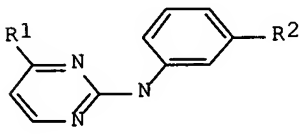
G14 = alkyl <containing 1-6 C>
G16 = S
Patent location: claim 10

L83 ANSWER 23 OF 25 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 123:169650 MARPAT Full-text
TITLE: Preparation of N-(fluroralkoxyphenyl)-2-pyrimidineamines as drugs
INVENTOR(S): Zimmermann, Juerg
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9509852	A1	19950413	WO 1994-EP3149	19940921
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, NO, NZ, PL, RO, RU, SI, SK, TJ, TT, UA, UZ, VN				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5543520	A	19960806	US 1994-306333	19940915
CA 2148477	A1	19950413	CA 1994-2148477	19940921
AU 9476975	A	19950501	AU 1994-76975	19940921
AU 693804	B2	19980709		
EP 672040	A1	19950920	EP 1994-927633	19940921
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 08504834	T	19960528	JP 1995-510576	19940921

PRIORITY APPLN. INFO.: CH 1993-2966 19931001
CH 1994-2278 19940718
WO 1994-EP3149 19940921

OTHER SOURCE(S): CASREACT 123:169650
GI

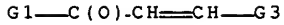


I

AB Title compds. [I; R1 = (N-oxido) 4-pyridyl, 3-indolyl, isoquinolyl, thienyl, pyrrolyl; R2 = fluoroalkoxy] were prepared as protein kinase C and tyrosine kinase inhibitors, etc. Thus, 3-(F2HCF2CO)C6H4NH2 was condensed with H2NCN and the guanidine product cyclocondensed with R1COCH:CHNMe2 (R1 = 4-pyridyl)

to give I (R1 = 4-pyridyl, R2 = OCF2CHF2). I had IC50 of .apprx.0.1 to 9μmol/L against protein kinase C in vitro.

MSTR 2



G1 = thienyl
G3 = loweralkylamino
Derivative: or salts
Patent location: claim 14

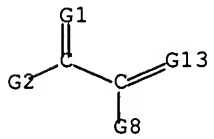
L83 ANSWER 24 OF 25 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 117:69570 MARPAT Full-text
TITLE: Preparation of 1-aryl-3-hydroxylamino-2-propen-1-ones and analogs as 5-lipoxygenase inhibitors
INVENTOR(S): Magolda, Ronald L.; Wright, Stephen W.
PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Co., USA
SOURCE: U.S., 11 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5110831	A	19920505	US 1990-621152	19901130

PRIORITY APPLN. INFO.: US 1990-621152 19901130

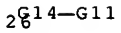
AB R1C(:X)CR3:CR4NR5OR7 [R1 = (cyclo)alkyl, OH, alkoxy, NH2, naphthyl, pyridyl, furyl, thienyl, (substituted) Ph, etc.; R3, R4 = H, groups cited for R1; or R3R4 = atoms to complete a ring; R5 = H, Ph, PhCH2, (cyclo)alkyl, etc.; R7 = H, COR8, SO2R8, cation; R8 = groups cited for R1; X = O, S] were prepared thus, 4-(PhH2CO)C6H4COMe was refluxed with Me2NCH(OMe)2 and the product condensed with HONHMe to give 4-RC6H4COCH:CHN(OH)Me (I; R = OCH2Ph). I (R = Ph) had IC50 of 0.06 μM against 5-lipoxygenase in vitro.

MSTR 2A

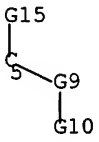


G1 = O
G2 = thienyl
G9 = NH

G10 = 26



G13 = 5



G14 = C(O)
Derivative: and pharmaceutically acceptable salts
Patent location: disclosure
Stereochemistry: and stereoisomers

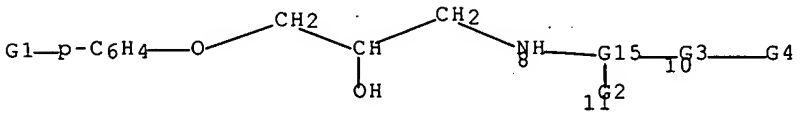
L83 ANSWER 25 OF 25 MARPAT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 83:131629 MARPAT Full-text
TITLE: 1-Phenoxy-3-aminopropan-2-ol derivatives
INVENTOR(S): Raabe, Thomas; Graewinger, Otto; Scholtholt, Josef; Nitz, Rolf E.; Schraven, Eckhard
PATENT ASSIGNEE(S): Cassella Farbwerke Mainkur A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 53 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2458738	A1	19750626	DE 1974-2458738	19741212
NL 7416375	A	19750624	NL 1974-16375	19741216
JP 50095283	A	19750729	JP 1974-145066	19741219
AU 7476662	A	19760624	AU 1974-76662	19741219
GB 1443488	A	19760721	GB 1974-54909	19741219
ES 433129	A1	19770216	ES 1974-433129	19741219
ES 433130	A1	19770216	ES 1974-433130	19741219
ES 433128	A1	19770301	ES 1974-433128	19741219
CH 603598	A5	19780831	CH 1974-16966	19741219
CH 605825	A5	19781013	CH 1974-16967	19741219
CH 605826	A5	19781013	CH 1974-16968	19741219
RO 68394	A1	19810622	RO 1974-80868	19741219
RO 68396	A1	19810730	RO 1974-80869	19741219
RO 68395	A1	19820706	RO 1974-80867	19741219
PL 98633	B1	19780531	PL 1974-176695	19741220
PRIORITY APPLN. INFO.:			LU 1973-69042	19731220

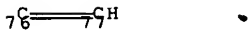
GI For diagram(s), see printed CA Issue.
AB Pyrimidines I (R = 2-OEt, 4-OBu, 4-NHAc, 4-OC5H11, 2-Cl, 4-Cl, 4-OMe, H, 4-OPr, 4-OCHMe2, 2-OMe, 3-OBu, 2-F, 4-OC8H17, 4-CMe3, 3-Cl, 3-OMe, 4-Br, 4-OEt, 4-OCH2Ph; X = CMe:CHCO) were prepared by treating II with

RC6H4OCH2CH(OH)CH2NH2 and were reduced to I (X = CHMeCH2CHOH). I are β-sympatholytics. Thus I (X = CHMeCH2CHOH, R = 4-OPr) had a β1-receptor blocking ED50 of 0.0036 mg/kg and a β2-receptor blocking ED50 of 0.48 mg/kg i.v. in dogs.

MSTR 1



G3 = C(O)
G4 = 2-thienyl
G15 = 76-8 77-10 76-11



Patent location: claims
Note: record may include structures from disclosure

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=> d his full

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L2           37 SEA SSS SAM L1
                D STAT QUE L2
L3          676 SEA SSS FUL L1
                SAVE TEMP L3 LAM287STR3L/A

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L4          413 SEA ABB=ON  PLU=ON  L3

     FILE 'REGISTRY' ENTERED AT 16:33:20 ON 04 JAN 2007
L5              STRUCTURE UPLOADED
L6            6 SEA SUB=L3 SSS SAM L5
                D SCA
L7          159 SEA SUB=L3 SSS FUL L5
                SAVE TEMP L7 LAM287STR5L/A

     FILE 'CAPLUS' ENTERED AT 16:36:19 ON 04 JAN 2007
L8          124 SEA ABB=ON  PLU=ON  L7

     FILE 'REGISTRY' ENTERED AT 16:36:26 ON 04 JAN 2007
L9            6 SEA ABB=ON  PLU=ON  L7 AND Z/BI
                D SCA
L10           2 SEA ABB=ON  PLU=ON  L7 AND 1Z/BI
L11          13 SEA ABB=ON  PLU=ON  L7 AND 2Z/BI
L12           0 SEA ABB=ON  PLU=ON  L7 AND 3Z/BI
L13          18 SEA ABB=ON  PLU=ON  (L9 OR L10 OR L11)
                D SCA

     FILE 'STNGUIDE' ENTERED AT 16:40:10 ON 04 JAN 2007

     FILE 'REGISTRY' ENTERED AT 16:43:11 ON 04 JAN 2007
L14             STRUCTURE UPLOADED
L15           0 SEA SUB=L7 SSS SAM L14
L16           0 SEA SUB=L7 SSS FUL L14
L17     6787059 SEA ABB=ON  PLU=ON  STEREOSEARCH/FS
L18          38 SEA ABB=ON  PLU=ON  L7 AND L17
L19           0 SEA ABB=ON  PLU=ON  L13 NOT L18
L20          20 SEA ABB=ON  PLU=ON  L18 NOT L13
                D SCA

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L21           9 SEA ABB=ON  PLU=ON  L13

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     FILE 'CAPLUS' ENTERED AT 16:59:44 ON 04 JAN 2007
L22      273570 SEA ABB=ON  PLU=ON  ?STEREO?/BI
L23      253224 SEA ABB=ON  PLU=ON  CIS?/BI
L24     6004686 SEA ABB=ON  PLU=ON  ?TRANS?/BI
L25           6 SEA ABB=ON  PLU=ON  L8 AND L22
L26           4 SEA ABB=ON  PLU=ON  L8 AND L23
L27          22 SEA ABB=ON  PLU=ON  L8 AND L24
L28          25 SEA ABB=ON  PLU=ON  (L25 OR L26 OR L27)
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                D SCA
L29           15 SEA ABB=ON  PLU=ON  L20
L30           11 SEA ABB=ON  PLU=ON  L29 NOT (L21 OR L25)

     FILE 'REGISTRY' ENTERED AT 17:08:07 ON 04 JAN 2007
L31               ANALYZE PLU=ON  L7 1- LC :      14 TERMS
                  D
L32               ANALYZE PLU=ON  L13 1- LC :      6 TERMS
                  D

     FILE 'CASREACT' ENTERED AT 17:09:40 ON 04 JAN 2007
L33           51 SEA ABB=ON  PLU=ON  L7

     FILE 'CAPLUS' ENTERED AT 17:11:11 ON 04 JAN 2007
L34           51 SEA ABB=ON  PLU=ON  L33
L35            3 SEA ABB=ON  PLU=ON  L22 AND L34
L36            0 SEA ABB=ON  PLU=ON  L35 NOT (L21 OR L25)

     FILE 'STNGUIDE' ENTERED AT 17:12:20 ON 04 JAN 2007
                  D SCA L13

     FILE 'REGISTRY' ENTERED AT 17:13:10 ON 04 JAN 2007

     FILE 'STNGUIDE' ENTERED AT 17:13:33 ON 04 JAN 2007

     FILE 'REGISTRY' ENTERED AT 17:13:45 ON 04 JAN 2007
                  D L5
L37               STRUCTURE UPLOADED
L38            2 SEA SUB=L7 SSS SAM L37
                  D SCA
L39            9 SEA SUB=L7 SSS FUL L37
                  D SCA

     FILE 'CAPLUS' ENTERED AT 17:16:48 ON 04 JAN 2007
L40            7 SEA ABB=ON  PLU=ON  L39
L41           16 SEA ABB=ON  PLU=ON  L21 OR L25 OR L40
                  D COST
L42               ANALYZE PLU=ON  L8 1- RN :   10302 TERMS
                  D

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L43            1 SEA ABB=ON  PLU=ON  34772-98-0
                  D SCA
L44            1 SEA ABB=ON  PLU=ON  4637-24-5
                  D SCA
L45            1 SEA ABB=ON  PLU=ON  88-15-3
                  D SCA
L46            1 SEA ABB=ON  PLU=ON  1201-93-0
                  D SCA
L47            1 SEA ABB=ON  PLU=ON  17168-45-5
                  D SCA
L48          158 SEA ABB=ON  PLU=ON  L7 NOT L43

     FILE 'CAPLUS' ENTERED AT 17:22:03 ON 04 JAN 2007
L49           84 SEA ABB=ON  PLU=ON  L48
L50               ANALYZE PLU=ON  L49 1- RN :    8014 TERMS
                  D

     FILE 'REGISTRY' ENTERED AT 17:22:40 ON 04 JAN 2007
L51            1 SEA ABB=ON  PLU=ON  4637-24-5
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                D SCA

     FILE 'BEILSTEIN' ENTERED AT 17:23:59 ON 04 JAN 2007
L52             0 SEA SSS SAM L37
L53             1 SEA SSS FUL L37

     FILE 'MARPAT' ENTERED AT 17:25:07 ON 04 JAN 2007
L54             1 SEA SSS SAM L37
L55            10 SEA SSS FUL L37

     FILE 'WPIX' ENTERED AT 17:25:53 ON 04 JAN 2007
L56             0 SEA SSS SAM L37
L57             1 SEA SSS FUL L37
L58             3 SEA ABB=ON  PLU=ON  L57/DCR
                  SEL SDRN,SDCN,DCSE L57
L59             3 SEA ABB=ON  PLU=ON  (RADOK2/DCR,DCN,DRN,DCRE OR 873835-0-0-0/DC
                  R,DCN,DRN,DCRE)

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     FILE 'CAPLUS' ENTERED AT 17:28:25 ON 04 JAN 2007
L60            78 SEA ABB=ON  PLU=ON  KOGAMI K?/AU
L61             5 SEA ABB=ON  PLU=ON  HAYASHIZAKA N?/AU
L62           421 SEA ABB=ON  PLU=ON  SATAKE S?/AU
L63             2 SEA ABB=ON  PLU=ON  FUSEYA I?/AU
L64            37 SEA ABB=ON  PLU=ON  KAGANO H?/AU
L65             1 SEA ABB=ON  PLU=ON  L60 AND L61 AND L62 AND L63 AND L64
                  D SCA
L66             2 SEA ABB=ON  PLU=ON  L60 AND (L61 OR L62 OR L63 OR L64)
L67             1 SEA ABB=ON  PLU=ON  L61 AND (L62 OR L63 OR L64)
L68             4 SEA ABB=ON  PLU=ON  L62 AND (L63 OR L64)
L69             1 SEA ABB=ON  PLU=ON  L63 AND L64
L70             5 SEA ABB=ON  PLU=ON  (L66 OR L67 OR L68 OR L69)
L71             1 SEA ABB=ON  PLU=ON  (L60 OR L61 OR L62 OR L63 OR L64) AND (L21
                  OR L25 OR L40)
L72            10 SEA ABB=ON  PLU=ON  L55
L73             1 SEA ABB=ON  PLU=ON  (L60 OR L61 OR L62 OR L63 OR L64) AND L72

     FILE 'WPIX' ENTERED AT 17:31:19 ON 04 JAN 2007
L74             4 SEA ABB=ON  PLU=ON  (L66 OR L67 OR L68 OR L69)
L75             1 SEA ABB=ON  PLU=ON  (L60 OR L61 OR L62 OR L63 OR L64) AND (L58
                  OR L59)

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L76             0 SEA ABB=ON  PLU=ON  L70

     FILE 'STNGUIDE' ENTERED AT 17:32:38 ON 04 JAN 2007

     FILE 'REGISTRY' ENTERED AT 17:33:14 ON 04 JAN 2007

     FILE 'CAPLUS' ENTERED AT 17:33:19 ON 04 JAN 2007
                D STAT QUE L65
                D STAT QUE L70
                D STAT QUE L71
L77             5 SEA ABB=ON  PLU=ON  L65 OR L70 OR L71

     FILE 'MARPAT' ENTERED AT 17:34:02 ON 04 JAN 2007
L78             1 SEA ABB=ON  PLU=ON  L73

     FILE 'WPIX' ENTERED AT 17:34:38 ON 04 JAN 2007
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                D STAT QUE L74
                D STAT QUE L75
L79           4 SEA ABB=ON  PLU=ON  (L74 OR L75)

     FILE 'STNGUIDE' ENTERED AT 17:35:11 ON 04 JAN 2007

     FILE 'CAPLUS, MARPAT, WPIX' ENTERED AT 17:35:23 ON 04 JAN 2007
L80           5 DUP REM L77 L78 L79 (5 DUPLICATES REMOVED)
                      ANSWERS '1-5' FROM FILE CAPLUS
                D IBIB ABS HITIND HITSTR L80 1-5

     FILE 'REGISTRY' ENTERED AT 17:35:54 ON 04 JAN 2007

     FILE 'CAPLUS' ENTERED AT 17:35:57 ON 04 JAN 2007
                D STAT QUE L21
                D STAT QUE L25
                D STAT QUE L40
L81          15 SEA ABB=ON  PLU=ON  (L21 OR L25 OR L40) NOT L77

     FILE 'BEILSTEIN' ENTERED AT 17:36:43 ON 04 JAN 2007
                D STAT QUE L53

     FILE 'WPIX' ENTERED AT 17:37:01 ON 04 JAN 2007
                D STAT QUE L58
                D STAT QUE L59
L82           2 SEA ABB=ON  PLU=ON  (L58 OR L59) NOT L79

     FILE 'STNGUIDE' ENTERED AT 17:37:52 ON 04 JAN 2007

     FILE 'CAPLUS, WPIX, BEILSTEIN, MARPAT' ENTERED AT 17:38:11 ON 04 JAN 2007
L83          25 DUP REM L81 L82 L53 L55 (3 DUPLICATES REMOVED)
                      ANSWERS '1-15' FROM FILE CAPLUS
                      ANSWER '16' FROM FILE BEILSTEIN
                      ANSWERS '17-25' FROM FILE MARPAT
                D IBIB ABS HITIND HITSTR L83 1-15
                D IDE ALLREF L83 16
                D IBIB ABS QHIT L83 17-25


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:    3 JAN 2007  HIGHEST RN 916687-76-8
     DICTIONARY FILE UPDATES:   3 JAN 2007  HIGHEST RN 916687-76-8

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

       Please note that search-term pricing does apply when
       conducting SmartSELECT searches.

     REGISTRY includes numerically searchable data for experimental and
     predicted properties as well as tags indicating availability of
     experimental property data in the original document.  For information
     on property searching in REGISTRY, refer to:
```

http://www.cas.org/ONLINE/UG/regprops.html

FILE CAPLUS

FILE COVERS 1907 - 4 Jan 2007 VOL 146 ISS 2
FILE LAST UPDATED: 3 Jan 2007 (20070103/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jan 2, 2007 (20070102/UP).

FILE CASREACT

FILE CONTENT:1840 - 31 Dec 2006 VOL 146 ISS 1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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**********************************************************.
*                                                        *
*     CASREACT now has more than 10 million reactions    *
*                                                        *
**********************************************************
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BEILSTEIN
FILE LAST UPDATED ON JUNE 16, 2006

FILE COVERS 1771 TO 2006.
FILE CONTAINS 9,606,495 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search

for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
****

NEW

* ***PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.***
* ***NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.***

FILE MARPAT
FILE CONTENT: 1961-PRESENT VOL 146 ISS 1 (20061229/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 7138540 21 NOV 2006
DE 102005018025 02 NOV 2006
EP 1721898 15 NOV 2006
JP 2006310097 09 NOV 2006
WO 2006126581 30 NOV 2006
GB 2425654 01 NOV 2006
FR 2885527 17 NOV 2006
RU 2287007 10 NOV 2006
CA 2546348 11 NOV 2006

Expanded G-group definition display now available.

FILE WPIX
FILE LAST UPDATED: 2 JAN 2007 <20070102/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200701 <200701/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> YOU ARE IN THE NEW AND ENHANCED DERWENT WORLD PATENTS INDEX <<<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
PLEASE VISIT:
http://www.stn-international.de/training_center/patents/stn_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
http://scientific.thomson.com/support/patents/coverage/latestupdates/

PLEASE BE AWARE OF THE NEW IPC REFORM IN 2006, SEE
http://www.stn-international.de/stndatabases/details/ipc_reform.html and
http://scientific.thomson.com/media/scpdf/ipcrdwpi.pdf

>>> FOR DETAILS ON THE NEW AND ENHANCED DERWENT WORLD PATENTS INDEX
PLEASE SEE
http://www.stn-international.de/stndatabases/details/dwpi_r.html <<<

FILE MEDLINE
FILE LAST UPDATED: 3 Jan 2007 (20070103/UP). FILE COVERS 1950 TO DATE.

All regular MEDLINE updates from November 15 to December 16 have been added to MEDLINE, along with 2007 Medical Subject Headings (MeSH(R)) and 2007 tree numbers.

The annual reload will be available in early 2007.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE EMBASE
FILE COVERS 1974 TO 4 Jan 2007 (20070104/ED)

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BIOSIS
FILE COVERS 1969 TO DATE.
CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT
FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 3 January 2007 (20070103/ED)

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